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(FILE 'HOME' ENTERED AT 13:49:10 ON 03 MAY 2005)

FILE 'HCAPLUS' ENTERED AT 13:50:03 ON 03 MAY 2005

L1 E LAL G/AU
40 SEA ABB=ON PLU=ON ("LAL G"/AU OR "LAL G S"/AU OR "LAL G
SANKAR"/AU)
E MINNICH K/AU
L2 23 SEA ABB=ON PLU=ON ("MINNICH K"/AU OR "MINNICH KRISTEN E"/AU
OR "MINNICH KRISTEN ELAINE"/AU OR "MINNICH KRISTIN"/AU OR
"MINNICH KRISTIN E"/AU)
L3 4315 SEA ABB=ON PLU=ON (AIR (1A) PROD? AND CHEM?)/CS, PA
L4 3 SEA ABB=ON PLU=ON (L1 OR L2) AND PENTAFLUOR?

FILE 'REGISTRY' ENTERED AT 13:52:52 ON 03 MAY 2005

FILE 'HCAPLUS' ENTERED AT 13:52:54 ON 03 MAY 2005
L5 TRA L4 1- RN : 59 TERMS

FILE 'REGISTRY' ENTERED AT 13:52:54 ON 03 MAY 2005
L6 59 SEA ABB=ON PLU=ON L5

=> b hcap

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FILE COVERS 1907 - 3 May 2005 VOL 142 ISS 19
FILE LAST UPDATED: 2 May 2005 (20050502/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all 14 tot

L4 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:254460 HCAPLUS
DN 142:318761
ED Entered STN: 24 Mar 2005
TI Synthesis of **pentafluorosulfuranyl** substituted alkanes
IN Lal, Gauri Sankar; **Minnich, Kristen Elaine**
PA Air Products and Chemicals, Inc., USA
SO U.S., 8 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07C309-00
INCL 562824000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6870068	B1	20050322	US 2003-713230	20031114
PRAI	US 2003-713230		20031114		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6870068	ICM	C07C309-00
	INCL	562824000
US 6870068	NCL	562/824.000
	ECLA	C07C381/00

AB Addition of an SF5 group to organic compds. such as alkyl-substituted terminal alkenes, internal alkenes and cycloalkenes via the reaction with SF5Br is effected under liquid phase conditions and generally in the presence of a free radical initiator, preferably tri-Et borane. (SBrF5) was condensed with 1-octene at -78° in the presence of tri-Et borane to give 1-pentafluorosulfanyl-2-bromooctane mol. weight 276.

ST sulfurpentafluoride addn olefin triethyl borane

IT Condensation reaction
(pentafluorosulfuranyl addition to various alkenes)

IT Cycloalkadienes
Cycloalkenes
RL: RCT (Reactant); RACT (Reactant or reagent)
(pentafluorosulfuranyl addition to various alkenes)

IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(α-; pentafluorosulfuranyl addition to various alkenes)

IT 97-94-9, Triethyl borane
RL: CAT (Catalyst use); USES (Uses)
(pentafluorosulfuranyl addition to various alkenes)

IT 100-40-3, 4-Vinyl-1-cyclohexene 100-42-5, Styrene, reactions 106-92-3, Allyl glycidyl ether 110-83-8, Cyclohexene, reactions 111-66-0, 1-Octene 115-07-1, Propylene, reactions 115-11-7, Isobutylene, reactions 498-66-8, Norbornene 591-93-5, 1,4-Pentadiene 592-42-7, 1,5-Hexadiene 592-45-0, 1,4-Hexadiene 592-57-4, 1,3-Cyclohexadiene 613-31-0, Dihydroanthracene 628-41-1, 1,4-Cyclohexadiene 930-68-7, 2-Cyclohexen-1-one 931-88-4, Cyclooctene 1321-74-0, Divinylbenzene, reactions 1322-67-4, Dodecahydrophenanthrene 1521-51-3, 3-Bromo-1-cyclohexene 1541-23-7, 1,5-Heptadiene 3070-53-9, 1,6-Heptadiene 5675-22-9, 1,4-Heptadiene 7642-10-6, cis-3-Heptene 14686-14-7, trans-3-Heptene 14850-23-8, trans-4-Octene 15607-89-3, Sulfur bromide fluoride (SBrF5) 25264-93-1, Hexene 25339-53-1, Decene 25339-56-4, Heptene 25377-72-4, Pentene 25378-22-7, Dodecene 26856-35-9, Dihydrophenanthrene 29828-28-2, Dihydronaphthalene 31244-58-3, Octahydronaphthalene 848193-39-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(pentafluorosulfuranyl addition to various alkenes)

IT 848192-76-7P 848192-77-8P 848192-78-9P 848192-79-0P 848192-80-3P
848192-81-4P 848192-82-5P 848192-83-6P 848192-84-7P 848192-85-8P
848192-86-9P 848192-87-0P 848192-88-1P 848192-89-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(pentafluorosulfuranyl addition to various alkenes)

RE. CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; EP 0444822 B1 1994 HCAPLUS
- (2) Anon; DE 19748109 A1 1999 HCAPLUS
- (3) Ayt-Mohand, S; Organic Letters 2002, V4(17), P3013
- (4) Chern; US 6136838 A 2000 HCAPLUS
- (5) Coffman; US 3284496 A 1966 HCAPLUS
- (6) Dieter, L; Chem of Hypervalent Compounds 1999, P295
- (7) Lal; US 6479645 B1 2002 HCAPLUS
- (8) Nixon; Journal of Fluorine Chem 1998, V91, P13 HCAPLUS
- (9) Rolf, W; Amer Chem Soc 1994, P128
- (10) Terjeson; Journal of Fluorine Chemistry 1987, V35(4), P653 HCAPLUS
- (11) Winter; Journal of Fluorine Chem 1994, V66, P109 HCAPLUS
- (12) Winter; Journal of Fluorine Chem 2000, V102, P79 HCAPLUS
- (13) Winter; Journal of Fluorine Chem 2003, V122, P251 HCAPLUS
- (14) Winter, R; Inorganic Chem, J of Fluo Chem 2001, V107, P23 HCAPLUS

L4 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:658884 HCAPLUS

ED Entered STN: 15 Aug 2004

TI Synthesis of organic compounds containing the pentafluorosulfanyl (SF5) group

AU **Lal, G. Sankar; Minnich, Kristin**
 CS Air Products and Chemicals, Inc, Allentown, PA, 18195-1501, USA
 SO Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), ORGN-620 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69FTZ8
 DT Conference; Meeting Abstract
 LA English
 AB The development of synthetic methodologies for the introduction of the **pentafluorosulfuranyl** groups ("SF5") into organic compds. has been pursued with a considerable degree of interest. The SF5 group imparts unique properties to these organic compds. that include, inter alia, low surface energy, high chemical resistance, high thermal stability, high electronegativity, hydrophobicity, and high dielec. constant. The high electronegativity value of the SF5 group, 3.62 on the Pauling scale, and its greater electron withdrawing ability makes it an attractive alternative for the trifluoromethyl group ("CF3") found in many com. products. In our laboratory, we have developed novel techniques for the introduction of the SF5-group into a variety of substrates including alkenes, alkynes and aromatic compds. using SF5Br. The results of these studies will be presented.

L4 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:864404 HCAPLUS
 DN 137:353172
 ED Entered STN: 14 Nov 2002
 TI Preparation of silylethynylsulfur **pentafluoride** compounds
 IN Lal, Gauri Sankar; **Minnich, Kristen Elaine**
 PA Air Products and Chemicals, Inc., USA
 SO U.S., 6 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07F007-08
 INCL 532427000
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6479645	B1	20021112	US 2002-104214	20020322
EP 1346996	A1	20030924	EP 2003-6214	20030320
EP 1346996	B1	20041215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004035540	A2	20040205	JP 2003-77065	20030320
AT 284888	E	20050115	AT 2003-6214	20030320
PRAI US 2002-104214	A	20020322		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6479645	ICM	C07F007-08
	INCL	532427000
US 6479645	NCL	556/427.000; 252/299.010
	ECLA	C07F007/08C6D
EP 1346996	ECLA	C07F007/08C6D
JP 2004035540	FTERM	4H049/VN01; 4H049/VP01; 4H049/VQ47; 4H049/VR24; 4H049/VS04; 4H049/VT03; 4H049/VT05; 4H049/VT23; 4H049/VT24; 4H049/VT28; 4H049/VU24; 4H049/VU36; 4H049/VW02

AB Ethynylsilyl sulfur **pentafluoride** compds., e.g., (R)(R')(R'')Si-C.tplbond.C-SF5 [wherein R, R', R'', independently = (substituted) alkyl, (substituted) aryl], were prepared. For example, trimethylsilylacetylene was reacted with SF5Br to give 1-bromo-1-trimethylsilyl-2-**pentafluorosulfuranylene**, which upon elimination by treatment with KOH gives 44% 1-**pentafluorosulfuranyl**-2-trimethylsilylethyne.

ST silyl ethynyl sulfur **pentafluoride** compd prepn; fluoride ethynylsulfur compd prepn

IT 474668-30-9P 474668-31-0P 474668-33-2P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic)

preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of silylethynylsulfur **pentafluoride** compds.)

IT 103077-41-4P 474668-32-1P 474668-34-3P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(preparation of silylethynylsulfur **pentafluoride** compds.)

IT 1066-54-2, Trimethylsilylacetylene 15607-89-3 86318-61-8,
tert-Butyldimethylsilylacetylene 89343-06-6, Triisopropylsilylacetylene

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of silylethynylsulfur **pentafluoride** compds.)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; DE 0444822 1994
- (2) Anon; DE 19748109 1999 HCAPLUS
- (3) Canich, J; Inorg Chem 1985, V24, P3668 HCAPLUS
- (4) Chern; US 6136838 A 2000 HCAPLUS
- (5) Dowbenko; US 4749803 A 1988 HCAPLUS
- (6) Fory; US 4053497 A 1977 HCAPLUS
- (7) Hoover; J Am Chem Soc 1964, V29, P3567 HCAPLUS
- (8) Kovacina; Ind Eng Chem Prod Res Dev 1983, V22(2), P170 HCAPLUS
- (9) Matsui; US 5728319 A 1998 HCAPLUS
- (10) Matsui; US 5792386 A 1998 HCAPLUS
- (11) Singer; US 4652664 A 1987 HCAPLUS
- (12) Wessel, J; Chem Ber 1986, V119, P45

=> b home

FILE 'HOME' ENTERED AT 13:53:38 ON 03 MAY 2005

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=> d his full

(FILE 'HOME' ENTERED AT 13:49:10 ON 03 MAY 2005)

FILE 'HCAPLUS' ENTERED AT 13:50:03 ON 03 MAY 2005

L1 E LAL G/AU
40 SEA ABB=ON PLU=ON ("LAL G"/AU OR "LAL G S"/AU OR "LAL G
SANKAR"/AU)
E MINNICH K/AU
L2 23 SEA ABB=ON PLU=ON ("MINNICH K"/AU OR "MINNICH KRISTEN E"/AU
OR "MINNICH KRISTEN ELAINE"/AU OR "MINNICH KRISTIN"/AU OR
"MINNICH KRISTIN E"/AU)
L3 4315 SEA ABB=ON PLU=ON (AIR (1A) PROD? AND CHEM?)/CS, PA
L4 3 SEA ABB=ON PLU=ON (L1 OR L2) AND PENTAFLUOR?
D SCA

FILE 'REGISTRY' ENTERED AT 13:52:52 ON 03 MAY 2005

FILE 'HCAPLUS' ENTERED AT 13:52:54 ON 03 MAY 2005

L5 TRA L4 1- RN : 59 TERMS

FILE 'REGISTRY' ENTERED AT 13:52:54 ON 03 MAY 2005

L6 59 SEA ABB=ON PLU=ON L5
L7 STR
L8 50 SEA SSS SAM L7
L9 4584 SEA SSS FUL L7
SAV TEM NWA0231F0/A L9
L10 STR
L11 50 SEA SSS SAM L10
D QUE STA L11
L12 1188 SEA SSS FUL L10
SAV TEM NWA0231F1/A L12

FILE 'HCAPLUS' ENTERED AT 14:16:18 ON 03 MAY 2005

L13 673 SEA ABB=ON PLU=ON L9 (L) RACT+NT/RL
L14 65 SEA ABB=ON PLU=ON L12 (L) PREP+NT/RL
L15 2 SEA ABB=ON PLU=ON L13 AND L14
L16 0 SEA ABB=ON PLU=ON L15 AND (L1 OR L2 OR L3)
L17 4 SEA ABB=ON PLU=ON L9 AND L12
L18 0 SEA ABB=ON PLU=ON L17 AND (L1 OR L2 OR L3)
D SCA L17
L19 4 SEA ABB=ON PLU=ON L15 OR L17

FILE 'CASREACT' ENTERED AT 14:18:59 ON 03 MAY 2005

L20 STR
L21 0 SEA SSS SAM L20 (0 REACTIONS)
L22 0 SEA SSS FUL L20 (0 REACTIONS)
L23 STR
L24 0 SEA SSS SAM L23 (0 REACTIONS)
L25 75 SEA SSS FUL L23 (314 REACTIONS)
E LAL G/AU
L26 29 SEA ABB=ON PLU=ON ("LAL G"/AU OR "LAL G S"/AU OR "LAL G
SANKAR"/AU OR "LAL GAURI S"/AU OR "LAL GAURI SANKAR"/AU)
E MINNICH K/AU
L27 127 SEA ABB=ON PLU=ON (AIR (1A) PROD? AND CHEM?)/CS, PA
L28 0 SEA ABB=ON PLU=ON L25 AND (L26 OR L27)
L29 QUE ABB=ON PLU=ON PY<=2003 OR AY<=2003 OR PRY<=2003 OR
PD<20031114 OR AD<20031114 OR PRD<20031114
L30 75 SEA ABB=ON PLU=ON L25 AND L29
D QUE STA L22
L31 STR L23
D QUE L31
L32 STR L31
L33 0 SEA SUB=L25 SSS SAM L32 (0 REACTIONS)
L34 STR L32
L35 0 SEA SUB=L25 SSS SAM L34 (0 REACTIONS)
D QUE STA L35
L36 STR L34
L37 STR L36
L38 16 SEA SUB=L25 SSS FUL L37 (36 REACTIONS)

Search done by Noble Jarrell

L39 0 SEA ABB=ON PLU=ON L38 AND (L26 OR L27)
 L40 STR
 L41 1 SEA SSS SAM L40 (1 REACTIONS)
 D SCA
 L42 STR L40
 L43 0 SEA SSS SAM L42 (0 REACTIONS)
 D QUE STA L43
 L44 22 SEA SSS FUL L42 (44 REACTIONS)
 L45 16 SEA ABB=ON PLU=ON L38 AND L29
 L46 21 SEA ABB=ON PLU=ON L44 AND L29
 L47 36 SEA ABB=ON PLU=ON (L45 OR L46)

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STRUCTURE FILE UPDATES: 2 MAY 2005 HIGHEST RN 849658-68-0
 DICTIONARY FILE UPDATES: 2 MAY 2005 HIGHEST RN 849658-68-0

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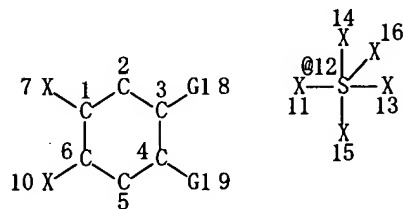
 *
 * The CA roles and document type information have been removed from *
 * the IDE default display format and the ED field has been added, *
 * effective March 20, 2005. A new display format, IDERL, is now *
 * available and contains the CA role and document type information. *
 *

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Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que sta 19

L7 STR



VAR G1=12/X

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

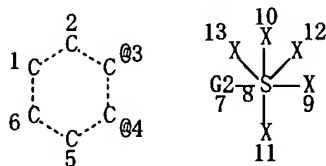
STEREO ATTRIBUTES: NONE

L9 4584 SEA FILE=REGISTRY SSS FUL L7

100.0% PROCESSED 20578 ITERATIONS
SEARCH TIME: 00.00.01

4584 ANSWERS

=> d que sta l12
L10 STR



VAR G2=3/4
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ELEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L12 1188 SEA FILE=REGISTRY SSS FUL L10

100.0% PROCESSED 1365 ITERATIONS
SEARCH TIME: 00.00.01

1188 ANSWERS

=> b hcap
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FILE COVERS 1907 - 3 May 2005 VOL 142 ISS 19
FILE LAST UPDATED: 2 May 2005 (20050502/ED)

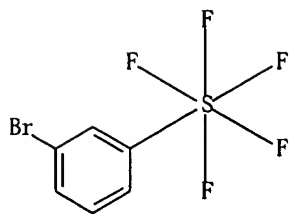
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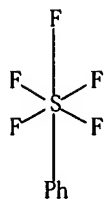
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L19 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:462899 HCAPLUS
DN 141:173955
ED Entered STN: 09 Jun 2004
TI A New Synthesis of Pentafluorosulfanylbenzene
AU Sergeeva, Tatiana A.; Dolbier, William R., Jr.
CS Department of Chemistry, University of Florida, Gainesville, FL, 32611, USA
S0 Organic Letters (2004), 6(14), 2417-2419

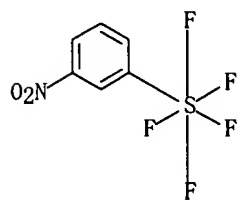
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 25-22 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 141:173955
AB A new and convenient three-step synthesis of pentafluorosulfanylbenzene from 1,4-cyclohexadiene with an overall yield of >70% is reported along with a number of derivatization reactions.
ST pentafluorosulfanylbenzene prepn reaction; benzene pentafluorosulfanyl prepn reaction
IT 628-41-1, 1,4-Cyclohexadiene 13780-57-9, Chloropentafluorosulfur
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and reactions of pentafluorosulfanylbenzene)
IT 672-30-0P 2557-81-5P 2613-26-5P
2993-22-8P 89415-83-8P 654671-65-5P
735331-67-6P
RL: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of pentafluorosulfanylbenzene)
IT 1736-99-8P 159727-25-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of pentafluorosulfanylbenzene)
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Ait-Mohand, S; Org Lett 2002, V4, P3013
(2) Bowden, R; PCT Int Appl 2002
(3) Bowden, R; Tetrahedron 2000, V56, P3399 HCAPLUS
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(8) Case, J; J Chem Soc 1961, P2066 HCAPLUS
(9) Chambers, R; Chem Commun 1999, P883 HCAPLUS
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(12) Dolbier, W; Chim Oggi 2003, V21, P66 HCAPLUS
(13) Duan, J; Synlett 1999, P1245 HCAPLUS
(14) Eaton, D; J Am Chem Soc 1963, V85, P1310 HCAPLUS
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(16) Fokin, A; Russ Chem Bull 1996, V45, P2804
(17) Hoover, F; J Org Chem 1964, V29, P3567 HCAPLUS
(18) Klauck, A; Angew Chem, Int Ed Engl 1994, V33, P93
(19) Ou, X; J Fluorine Chem 2000, V101, P279 HCAPLUS
(20) Riemschneider, R; Chem Ber 1955, V88, P1442 HCAPLUS
(21) Sheppard, W; J Am Chem Soc 1962, V84, P3064
(22) Sheppard, W; J Am Chem Soc 1962, V84, P3064
(23) Sheppard, W; J Am Chem Soc 1962, V84, P3072 HCAPLUS
(24) Sipyagin, A; J Fluorine Chem 2001, V112, P287 HCAPLUS
(25) Taft, R; J Am Chem Soc 1963, V85, P709 HCAPLUS
(26) Winter, R; Inorganic Fluorine Chemistry-Toward the 21st Century 1994, V555, P128 HCAPLUS
(27) Winter, R; J Fluorine Chem 2004, V125, P549 HCAPLUS
IT 672-30-0P 2557-81-5P 2613-26-5P
2993-22-8P 654671-65-5P 735331-67-6P
RL: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of pentafluorosulfanylbenzene)
RN 672-30-0 HCAPLUS
CN Sulfur, (3-bromophenyl)pentafluoro-, (OC-6-21)- (9CI) (CA INDEX NAME)



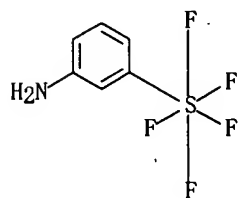
RN 2557-81-5 HCAPLUS
 CN Sulfur, pentafluorophenyl-, (OC-6-21)- (9CI) (CA INDEX NAME)



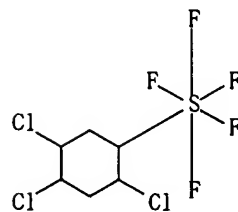
RN 2613-26-5 HCAPLUS
 CN Sulfur, pentafluoro(3-nitrophenyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



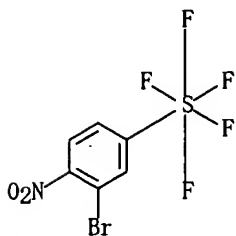
RN 2993-22-8 HCAPLUS
 CN Sulfur, (3-aminophenyl)pentafluoro-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 654671-65-5 HCAPLUS
 CN Sulfur, pentafluoro(2,4,5-trichlorocyclohexyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)

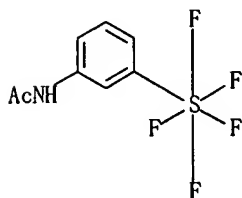


RN 735331-67-6 HCAPLUS
 CN Sulfur, (3-bromo-4-nitrophenyl)pentafluoro-, (OC-6-21)- (9CI) (CA INDEX NAME)

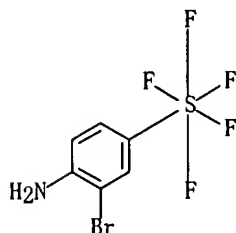


IT 1736-99-8P 159727-25-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and reactions of pentafluorosulfanylbenzene)

RN 1736-99-8 HCAPLUS
 CN Sulfur, [3-(acetamino)phenyl]pentafluoro-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 159727-25-0 HCAPLUS
 CN Sulfur, (4-amino-3-bromophenyl)pentafluoro-, (OC-6-21)- (9CI) (CA INDEX NAME)



L19 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:101125 HCAPLUS
 DN 140:163466
 ED Entered STN: 08 Feb 2004
 TI Stereoselective method and catalysts for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compounds
 IN Dolbier, William R., Jr.; Ait-Mohand, Samia
 PA University of Florida, USA
 SO PCT Int. Appl., 16 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07C381-00
 CC 23-12 (Aliphatic Compounds)
 Section cross-reference(s): 21, 67

FAN. CNT 1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004011422	A1	20040205	WO 2003-US24836	20030724

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
 PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
 TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 US 2004106827 A1 20040603 US 2003-627831 20030724
 PRAI US 2002-399044P P 20020725
 US 2003-448831P P 20030221

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004011422	ICM	C07C381-00
US 2004106827	NCL	562/826.000

OS CASREACT 140:163466
 AB A convenient, regiospecific and highly stereoselective addition of SF5Cl in
 high yield to a variety of alkenes (e.g., 1-heptene into
 2-chloro-1-pentafluorosulfanylheptane) and alkynes is presented using
 organoboron (e.g., triethylboron) catalysts.

ST chloropentafluorosulfanylheptane prepn pentafluorosulfanyl chloride
 catalytic stereoselective addn heptene; pentafluorosulfanyl moiety
 incorporation alkene; alkyne pentafluorosulfanyl moiety incorporation
 IT Aromatization
 Drying
 Elimination reaction
 Hydrolysis
 Oxidation
 (in the preparation of pentafluorosulfanyl-substituted aromatic compds.)

IT Boranes
 RL: CAT (Catalyst use); USES (Uses)
 (organo-; catalysts in a stereoselective method for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
 IT Alkanes, preparation
 Aromatic hydrocarbons, preparation
 Cycloalkanes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (pentafluorosulfanyl-substituted; stereoselective method and catalysts
 for incorporation of pentafluorosulfanyl substituents into aliphatic and
 aromatic compds.)

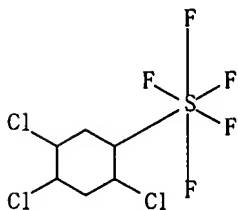
IT Stereochemistry
 (stereoselective method and catalysts for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
 IT Alkenes, reactions
 Alkynes
 Cycloalkenes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compds.)

IT Addition reaction catalysts
 (stereoselective; organoborons in a stereoselective method for
 incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic
 compds.)
 IT Addition reaction
 (stereoselective; stereoselective method and catalysts for
 incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic
 compds.)

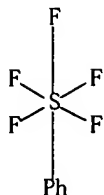
IT 141-52-6, Sodium ethoxide
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (base; stereoselective method and catalysts for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
 IT 97-94-9, Triethylboron 280-64-8, 9-Borabicyclo[3.3.1]nonane
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst in a stereoselective method for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compds.)

IT 75-09-2, Dichloromethane, uses 110-54-3, Hexane, uses
 RL: NUU (Other use, unclassified); USES (Uses)

- (solvent; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 7732-18-5, Water, uses
 RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses)
 (solvent; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 460745-77-1P
 RL: BYP (Byproduct); PREP (Preparation)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 108-05-4, Vinyl acetate, reactions 109-49-9, 5-Hexen-2-one 110-83-8, Cyclohexene, reactions 111-66-0, 1-Octene 536-74-3, Phenylacetylene 558-37-2 592-41-6, 1-Hexene, reactions 592-57-4, 1,3-Cyclohexadiene 622-97-9 629-05-0, 1-Octyne 760-21-4 1942-45-6, 4-Octyne 1968-40-7, 4-Pentenoic acid ethyl ester 13019-22-2, 9-Decen-1-ol 13780-57-9 14850-23-8 50816-18-7, 9-Decen-1-ol acetate 62871-09-4 89415-83-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 654671-65-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 1735-68-8P 2557-81-5P 334543-90-7P 334543-91-8P 334543-92-9P 460745-71-5P 460745-72-6P 460745-73-7P 460745-74-8P 460745-75-9P 460745-76-0P 460745-78-2P 460745-79-3P 461026-46-0P 654671-62-2P 654671-63-3P 654671-64-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- RE. CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
 (1) Ait-Mohand, S; ORG LETT 2002, V4(17), P3013
 (2) Coffman, D; US 3102903 A 1963 HCAPLUS
 (3) Imperial Chemical Industries Ltd; GB 891552 A 1962 HCAPLUS
 (4) Imperial Chemical Industries Ltd; GB 905006 A 1962 HCAPLUS
 (5) Imperial Chemical Industries Ltd; GB 907648 A 1962 HCAPLUS
 (6) Sheppard, W; J AMC CHEM SOC 1962, V84, P3064
- IT 654671-65-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- RN 654671-65-5 HCAPLUS
 CN Sulfur, pentafluoro(2,4,5-trichlorocyclohexyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



- IT 2557-81-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- RN 2557-81-5 HCAPLUS
 CN Sulfur, pentafluorophenyl-, (OC-6-21)- (9CI) (CA INDEX NAME)



L19 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:311136 HCAPLUS
 DN 130:326798
 ED Entered STN: 21 May 1999
 TI A method for performing a chemical reaction
 IN Harston, Paul; Atherton, Malcolm John; Holmes, Robert G. G.; Chambers, Richard Dickinson; Spink, Robert
 PA British Nuclear Fuels PLC, UK
 SO PCT Int. Appl., 22 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM B01J019-00
 ICS C07B039-00
 CC 48-8 (Unit Operations and Processes)
 Section cross-reference(s): 47

FAN. CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9922857	A1	19990514	WO 1998-GB3285	19981105
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 9810107	A	19990416	ZA 1998-10107	19981105
CA 2304550	AA	19990514	CA 1998-2304550	19981105
AU 9911630	A1	19990524	AU 1999-11630	19981105
EP 1028801	A1	20000823	EP 1998-954568	19981105
R: DE, FR, GB				
JP 2001521816	T2	20011113	JP 2000-518778	19981105
US 6747178	B1	20040608	US 2000-530231	20001002
PRAI GB 1997-23260	A	19971105		
WO 1998-GB3285	W	19981105		

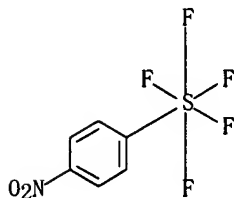
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9922857	ICM	B01J019-00
	ICS	C07B039-00
WO 9922857	ECLA	B01J019/00R; C07B039/00; C07C017/04+22/00; C07C045/46; C07C051/62+55/40; C07C067/307+69/716; C07C381/00
US 6747178	NCL	570/175.000
	ECLA	B01J019/00R; C07B039/00; C07C017/04+22/00; C07C045/46; C07C051/62+55/40; C07C067/307+69/716; C07C381/00

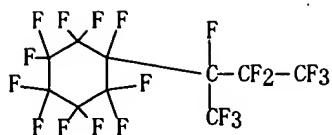
AB A method is provided for carrying out a chemical reaction between at least two fluids. The method includes providing resp. flow paths for the at least two fluids, where flow paths communicate with each other in a region in which the at least two fluids may contact each other, and flowing the at least two fluids along the flow paths such that in the region at least two fluids contact each other and a chemical reaction occurs between them; the region has a width perpendicular to the direction of flow in the range 10-10,000 μm . It was found that using a so-called "microreactor", that is a reactor having dimensions perpendicular to the flow direction of <10,000 μm , according to the method, improved control over a fluid chemical reaction can be achieved, which can result in significant improvements in reaction product yield and/or purity as well as other

benefits. The method was found to be particularly beneficial for fluorination reactions.

- ST fluorination microreactor system; reaction microreactor system
 IT Reactors
 (microreactors; system for performing chemical reactions, especially fluorination)
 IT Fluorination
 Reaction
 (system for performing chemical reactions, especially fluorination)
 IT 7727-37-9, Nitrogen, processes
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (fluorine in; system for performing chemical reactions, especially fluorination)
 IT **2613-27-6P**
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (in acetonitrile; system for performing chemical reactions, especially fluorination)
 IT 1526-28-9
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (in dry acetonitrile; system for performing chemical reactions, especially fluorination)
 IT 75-05-8, Acetonitrile, processes 75-09-2, Dichloromethane, processes
 141-97-9 543-20-4, Butanedioyl dichloride 7487-88-9, Sulfuric acid
 magnesium salt (1:1), processes 7681-49-4, Sodium fluoride (NaF),
 processes 7782-41-4, Fluorine, processes 131319-28-3 223791-47-7
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (system for performing chemical reactions, especially fluorination)
 IT 537-91-7
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC
 (Process); RACT (Reactant or reagent)
 (system for performing chemical reactions, especially fluorination)
 IT 1522-41-4P **132868-02-1P** 223791-48-8P 223915-29-5P
 223915-31-9P
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (system for performing chemical reactions, especially fluorination)
 IT 7664-39-3, Hydrogen fluoride, processes
 RL: REM (Removal or disposal); PROC (Process)
 (system for performing chemical reactions, especially fluorination)
 IT 7440-02-0, Nickel, uses
 RL: DEV (Device component use); USES (Uses)
 (tube; system for performing chemical reactions, especially fluorination)
 RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE
 (1) Central Research Laboratories; WO 9612541 A 1996 HCAPLUS
 IT **2613-27-6P**
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (in acetonitrile; system for performing chemical reactions, especially fluorination)
 RN 2613-27-6 HCAPLUS
 CN Sulfur, pentafluoro(4-nitrophenyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



- IT **132868-02-1P**
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (system for performing chemical reactions, especially fluorination)
 RN 132868-02-1 HCAPLUS
 CN Cyclohexane, 1,1,2,2,3,3,4,4,5,5,6-undecafluoro-6-[1,2,2,3,3,3-hexafluoro-1-(trifluoromethyl)propyl]- (9CI) (CA INDEX NAME)



L19 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1995:255415 HCAPLUS
 DN 122:58831
 ED Entered STN: 21 Dec 1994
 TI Process for the preparation of aryl- and heteroarylsulphurpentafluorides
 IN Williams, Alfred Glyn; Foster, Nicholas Russell
 PA Zeneca Ltd., UK
 SO PCT Int. Appl., 17 pp.
 CODEN: PIXXD2

DT Patent
 LA English
 IC ICM C07C381-00
 ICS C07D213-71
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 25

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9422817	A1	19941013	WO 1994-GB740	19940407
	W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9464343	A1	19941024	AU 1994-64343	19940407
	EP 693056	A1	19960124	EP 1994-912026	19940407
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08508476	T2	19960910	JP 1994-521880	19940407
PRAI	GB 1993-7245	A	19930407		
	WO 1994-GB740	W	19940407		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 9422817	ICM	C07C381-00
	ICS	C07D213-71

AB The process comprises reacting an aryldisulfide or heteroaryldisulfide with AgF₂ under anhydrous conditions at a temperature of $\geq 100^\circ$ and in the presence of a non-aqueous solvent whose b.p. is at or above the reaction temperature, said solvent being substantially stable under the reaction conditions. Reacting 4-nitrophenyldisulfide with AgF₂ in octane at 122-124° gave 4-nitrobenzenesulphurpentafluoride with 78% yield.

ST heteroarylsulphurpentafluoride prepn; heteroaryldisulfide silver difluoride reaction; aryldisulfide silver difluoride reaction; nitrobenzenesulphurpentafluoride prepn

IT 100-32-3 537-91-7 1155-00-6 2127-03-9 7783-95-1, Silver difluoride 159761-91-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for the preparation of aryl- and heteroarylsulphurpentafluorides)

IT 2613-26-5P 2613-27-6P 159761-89-4P 159761-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(process for the preparation of aryl- and heteroarylsulphurpentafluorides)

IT 111-65-9, Octane, uses 111-84-2, Nonane 306-94-5, Perfluorodecalin 358-21-4, Perfluoroethyl ether 375-45-1

RL: NUU (Other use, unclassified); USES (Uses)

(solvent; process for the preparation of aryl- and heteroarylsulphurpentafluorides)

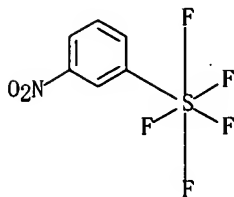
IT 2613-26-5P 2613-27-6P 159761-90-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(process for the preparation of aryl- and heteroarylsulphurpentafluorides)

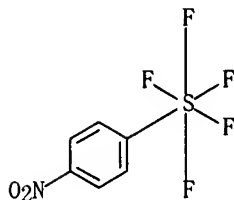
RN 2613-26-5 HCAPLUS

CN Sulfur, pentafluoro(3-nitrophenyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



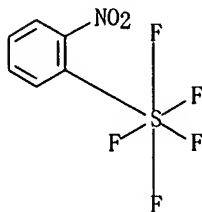
RN 2613-27-6 HCAPLUS

CN Sulfur, pentafluoro(4-nitrophenyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)



RN 159761-90-7 HCAPLUS

CN Sulfur, pentafluoro(2-nitrophenyl)-, (OC-6-21)- (9CI) (CA INDEX NAME)

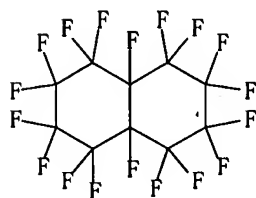


IT 306-94-5, Perfluorodecalin

RL: NUU (Other use, unclassified); USES (Uses)
(solvent; process for the preparation of aryl- and
heteroarylsulphurpentafluorides)

RN 306-94-5 HCAPLUS

CN Naphthalene, octadecafluorodecahydro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



=> b casre

FILE 'CASREACT' ENTERED AT 14:55:44 ON 03 MAY 2005
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Search done by Noble Jarrell

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 1 May 2005 VOL 142 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

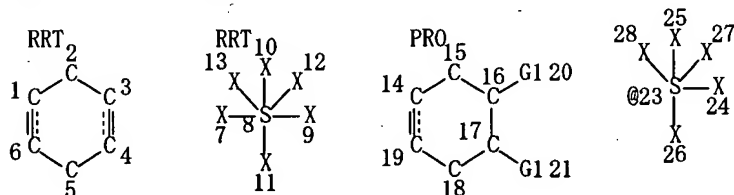
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que sta l22

L20 STR



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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

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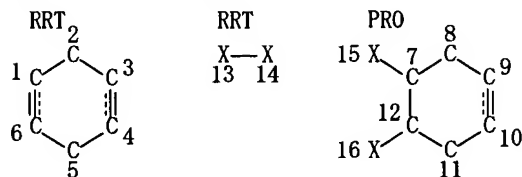
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=> d que sta l38

L23 STR



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DEFAULT ECLEVEL IS LIMITED

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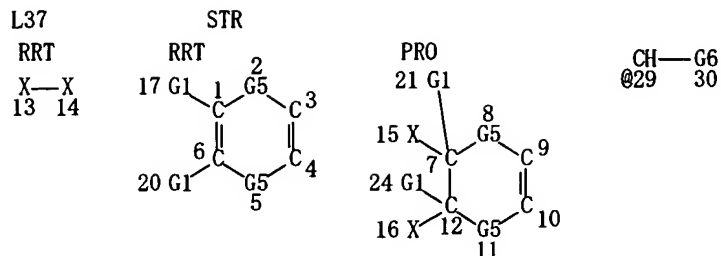
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NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

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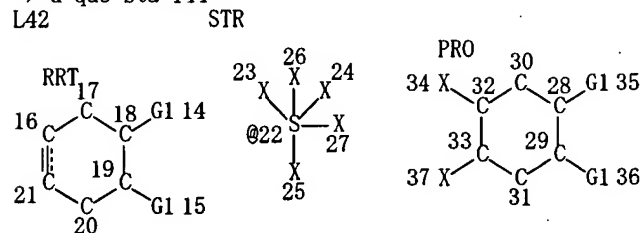
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 VAR G6=X/AK/O/S/CY/N
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
 L38 16 SEA FILE=CASREACT SUB=L25 SSS FUL L37 (36 REACTIONS)

100.0% DONE 262 VERIFIED 36 HIT RXNS 16 DOCS
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=> d que sta 144



VAR G1=22/X
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 16 28
 NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE
 L44 22 SEA FILE=CASREACT SSS FUL L42 (44 REACTIONS)

100.0% DONE 4479 VERIFIED 44 HIT RXNS 22 DOCS
 SEARCH TIME: 00.00.01

=> d bib abs ind crd retable 147 tot

L47 ANSWER 1 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 140:163466 CASREACT
 TI Stereoselective method and catalysts for incorporation of
 pentafluorosulfanyl substituents into aliphatic and aromatic compounds
 IN Dolbier, William R., Jr.; Ait-Mohand, Samia
 PA University of Florida, USA
 SO PCT Int. Appl., 16 pp.

Search done by Noble Jarrell

CODEN: PIXXD2

DT Patent

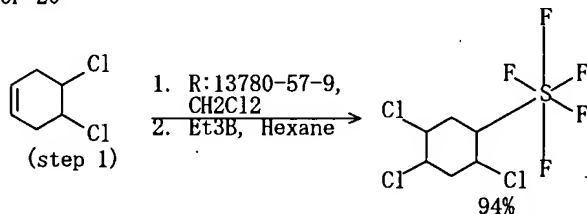
LA English

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004011422	A1	20040205	WO 2003-US24836	20030724
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2004106827	A1	20040603	US 2003-627831	20030724
PRAI	US 2002-399044P		20020725		
	US 2003-448831P		20030221		
AB	A convenient, regiospecific and highly stereoselective addition of SF5Cl in high yield to a variety of alkenes (e.g., 1-heptene into 2-chloro-1-pentafluorosulfanylheptane) and alkynes is presented using organoboron (e.g., triethylboron) catalysts.				
IC	ICM C07C381-00				
CC	23-12 (Aliphatic Compounds)				
	Section cross-reference(s): 21, 67				
ST	chloropentafluorosulfanylheptane prepn pentafluorosulfanyl chloride catalytic stereoselective addn heptene; pentafluorosulfanyl moiety incorporation alkene; alkyne pentafluorosulfanyl moiety incorporation				
IT	Aromatization				
	Drying				
	Elimination reaction				
	Hydrolysis				
	Oxidation				
	(in the preparation of pentafluorosulfanyl-substituted aromatic compds.)				
IT	Boranes				
	RL: CAT (Catalyst use); USES (Uses)				
	(organo-; catalysts in a stereoselective method for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	Alkanes, preparation				
	Aromatic hydrocarbons, preparation				
	Cycloalkanes				
	RL: SPN (Synthetic preparation); PREP (Preparation)				
	(pentafluorosulfanyl-substituted; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	Stereochemistry				
	(stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	Alkenes, reactions				
	Alkynes				
	Cycloalkenes				
	RL: RCT (Reactant); RACT (Reactant or reagent)				
	(stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	Addition reaction catalysts				
	(stereoselective; organoborons in a stereoselective method for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	Addition reaction				
	(stereoselective; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	141-52-6, Sodium ethoxide				
	RL: RGT (Reagent); RACT (Reactant or reagent)				
	(base; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)				
IT	97-94-9, Triethylboron 280-64-8, 9-Borabicyclo[3.3.1]nonane				
	RL: CAT (Catalyst use); USES (Uses)				

- (catalyst in a stereoselective method for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 75-09-2, Dichloromethane, uses 110-54-3, Hexane, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (solvent; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 7732-18-5, Water, uses
 RL: NUU (Other use, unclassified); REM (Removal or disposal); PROC (Process); USES (Uses)
 (solvent; stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 460745-77-1P
 RL: BYP (Byproduct); PREP (Preparation)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 108-05-4, Vinyl acetate, reactions 109-49-9, 5-Hexen-2-one 110-83-8, Cyclohexene, reactions 111-66-0, 1-Octene 536-74-3, Phenylacetylene 558-37-2 592-41-6, 1-Hexene, reactions 592-57-4, 1,3-Cyclohexadiene 622-97-9 629-05-0, 1-Octyne 760-21-4 1942-45-6, 4-Octyne 1968-40-7, 4-Pentenoic acid ethyl ester 13019-22-2, 9-Decen-1-ol 13780-57-9 14850-23-8 50816-18-7, 9-Decen-1-ol acetate 62871-09-4 89415-83-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 654671-65-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)
- IT 1735-68-8P 2557-81-5P 334543-90-7P 334543-91-8P 334543-92-9P 460745-71-5P 460745-72-6P 460745-73-7P 460745-74-8P 460745-75-9P 460745-76-0P 460745-78-2P 460745-79-3P 461026-46-0P 654671-62-2P 654671-63-3P 654671-64-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective method and catalysts for incorporation of pentafluorosulfanyl substituents into aliphatic and aromatic compds.)

RX(19) OF 20



RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Ait-Mohand, S	2002	4	3013	ORG LETT	
Coffman, D	1963			US 3102903 A	CAPLUS
Imperial Chemical Indus	1962			GB 891552 A	CAPLUS
Imperial Chemical Indus	1962			GB 905006 A	CAPLUS
Imperial Chemical Indus	1962			GB 907648 A	CAPLUS
Sheppard, W	1962	84	3064	J AMC CHEM SOC	

L47 ANSWER 2 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 140:4793 CASREACT

TI An efficient and highly stereoselective synthesis of gala-quercitol from 1,4-cyclohexadiene

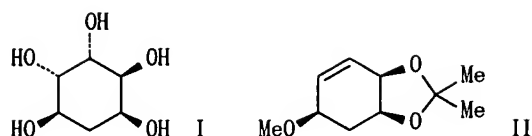
AU Baran, Arif; Secen, Hasan; Balci, Metin

CS Department of Chemistry, Ataturk University, Erzurum, 25240, Turk.

SO Synthesis (2003), (10), 1500-1502

CODEN: SYNTBF; ISSN: 0039-7881

PB Georg Thieme Verlag
 DT Journal
 LA English
 GI



AB Gala-Quercitol (I) was synthesized from 1,4-cyclohexadiene, in seven steps, in good yield. Reaction of 5,6-dibromo-2,2-dimethylhexahydro-1,3-benzodioxole, synthesized from 1,4-cyclohexadiene in three steps, with excess NaOMe gave II. Cis-Hydroxylation of the benzodioxole followed by acetylation with acetyl chloride gave 5-O-methyl-gala-quercitol tetraacetate from which I was obtained by hydrolysis and demethylation with aqueous HBr.

CC 24-5 (Alicyclic Compounds)

ST cyclohexadiene bromination; cyclohexene dibromide prepn dihydroxylation; bromocyclohexanediol prepn; quercitol prepn

IT Bromination

Dihydroxylation

Stereoselective synthesis

(stereoselective preparation of gala-quercitol via bromination of cyclohexadiene followed by cis-dihydroxylation, acetalation with dimethoxypropane, substitution, elimination, cis-dihydroxylation, acetylation, and deprotection)

IT 77-76-9, 2,2-Dimethoxypropane 628-41-1, 1,4-Cyclohexadiene

RL: RCT (Reactant); RACT (Reactant or reagent)

(stereoselective preparation of gala-quercitol via bromination of cyclohexadiene followed by cis-dihydroxylation, acetalation with dimethoxypropane, substitution, elimination, cis-dihydroxylation, acetylation, and deprotection)

IT 42846-36-6P 80409-81-0P 80446-29-3P 627878-70-0P 627878-71-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

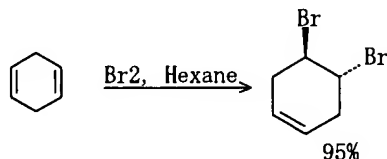
(stereoselective preparation of gala-quercitol via bromination of cyclohexadiene followed by cis-dihydroxylation, acetalation with dimethoxypropane, substitution, elimination, cis-dihydroxylation, acetylation, and deprotection)

IT 81369-62-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of gala-quercitol via bromination of cyclohexadiene followed by cis-dihydroxylation, acetalation with dimethoxypropane, substitution, elimination, cis-dihydroxylation, acetylation, and deprotection)

RX(1) OF 21



NOTE: stereoselective

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Ackermann, L	2000	56	2195	Tetrahedron	CAPLUS
Akbulut, N	1988	53	3338	J Org Chem	CAPLUS
Angelaud, R	1996	61	5202	J Org Chem	CAPLUS
Angyal, S	1981	101	209	Carbohydr Res	

Balci, M	1997	69	97	Pure Appl Chem	CAPLUS
de Sousa, S	2002	58	4643	Tetrahedron	CAPLUS
Desjardins, M	1999	1	621	J Chem Soc Perkin, T	
Dubreuil, D	1997	53	16747	Tetrahedron	CAPLUS
Gogek, C	1951	29	938	Can J Chem	CAPLUS
Haines, A	1998	39	4393	Tetrahedron Lett	CAPLUS
Kim, K	1998		1945	Chem Commun	CAPLUS
Lee, W	1999	10	4473	Tetrahedron:Asymmetr	CAPLUS
Maezaki, N	1999	40	3781	Tetrahedron Lett	CAPLUS
Mara, A	1998	308	435	Carbohydr Res	
Mara, A	1998	63	2039	J Org Chem	
McCasland, G	1965	20	11	Adv Carbohydr Chem	CAPLUS
McCasland, G	1961	83	2335	J Am Chem Soc	CAPLUS
Mehta, G	2000		2429	Chem Commun	CAPLUS
Mehta, G	2000	41	3509	Tetrahedron Lett	CAPLUS
Nakajima, M	1961	94	515	Chem Ber	
Ogawa, S	2001	20	703	J Carbohydr Chem	CAPLUS
Salamci, E	1997	62	2453	J Org Chem	CAPLUS
Salamci, E	1997	27	2223	Synth Commun	CAPLUS
Secen, H	1993		609	Synlett	CAPLUS
Secen, H	1990	31	1323	Tetrahedron Lett	CAPLUS
Secen, H	1993	17	108	Turk J Chem	CAPLUS
Sutbeyaz, Y	1988		1330	J Chem Soc, Chem Com	CAPLUS
Trost, B	1999	121	10834	J Am Chem Soc	CAPLUS
Trost, B	1999	40	219	Tetrahedron Lett	CAPLUS
Wibaut, J	1948	67	91	Recl Trav Chim Pays-	
Yadav, J	2001	66	8370	J Org Chem	CAPLUS
Yang, N	1984	106	7310	J Am Chem Soc	CAPLUS
Yoshizaki, H	1998	63	9339	J Org Chem	CAPLUS

L47 ANSWER 3 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 126:157179 CASREACT

TI Synthesis of fluorohydrocarbylsulfonates

IN Huang, Weiyuan; Xie, Yinbao

PA Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop.
Rep. China

SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 14 pp.

CODEN: CNXXEV

DT Patent

LA Chinese

FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1097191	A	19950111	CN 1993-112483	19930708
PRAI	CN 1993-112483		19930708		
AB	Title compds. were prepared by dehalosulfonation of fluorohaloalkanes or fluoroalkenes with MHSO ₃ or M ₂ S ₂ O ₅ (M = one valent metal or ammonium ion) in the presence of amines. Thus, reaction of CF ₂ ClCFC1 ₂ with NaHSO ₃ in DMF in the presence of BuNH ₂ gave 77% FC1CHCF ₂ SO ₃ Na.				
IC	ICM C07C303-32				
CC	23-12 (Aliphatic Compounds)				
ST	fluoroalkylsulfonate prepn				
IT	Alkanes, reactions				
	RL: RCT (Reactant); RACT (Reactant or reagent)				
	(halo; synthesis of fluorohydrocarbylsulfonates by dehalosulfonation of fluorohaloalkanes in presence of amines)				
IT	Amines, reactions				
	RL: RCT (Reactant); RACT (Reactant or reagent)				
	(synthesis of fluorohydrocarbylsulfonates by dehalosulfonation of fluorohaloalkanes in presence of amines)				
IT	76-13-1	79-38-9	109-73-9,	Butylamine, reactions	109-89-7,
	Diethylamine, reactions	110-89-4,	Piperidine, reactions	110-91-8,	
	Morpholine, reactions	116-15-4	121-44-8, reactions	123-75-1,	
	Pyrrolidine, reactions	124-73-2	354-51-8	354-65-4	355-75-9
	661-95-0	3916-24-3	7631-90-5	7681-57-4	160625-58-1
	186826-74-4				186826-72-2
	RL: RCT (Reactant); RACT (Reactant or reagent)				
	(synthesis of fluorohydrocarbylsulfonates)				
IT	377-30-0P	464-14-2P	13318-02-0P	160625-59-2P	

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

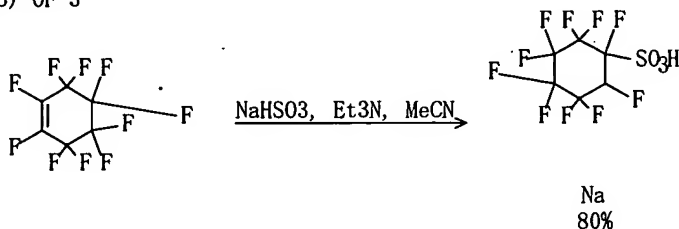
(synthesis of fluorohydrocarbylsulfonates)

IT 374-42-5P 186826-60-8P 186826-69-7P 186826-76-6P 186826-79-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of fluorohydrocarbylsulfonates)

RX(3) OF 3



L47 ANSWER 4 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 120:8228 CASREACT

TI Partially fluorinated enamines and their electrochemical fluorination

AU Moldavsky, D. D.; Kaurova, G. I.; Bispen, T. A.; Furin, G. G.

CS Inst. Appl. Chem., St. Petersburg, 197198, Russia

SO Journal of Fluorine Chemistry (1993), 63(3), 193-201

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

AB The reactions of hexafluoropropylene, its dimers and trimers, and perfluoro-1-ethylcyclohex-1-ene with secondary amines (dipropylamine, dibutylamine and diallylamine) have been shown to form enamines. The enamines were electrochem. fluorinated in anhydrous hydrogen fluoride. This paper reports the electrochem. fluorination data for the fluorination of tripropylamine, tributylamine, triamylamine and the partially fluorinated enamines. The structures of the products have been confirmed by ¹⁹F NMR and GC-MS methods.

CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 72

ST electrochem fluorination enamine partially fluorinated

IT Enamines

RL: RCT (Reactant); RACT (Reactant or reagent)

(partially fluorinated, electrochem. fluorination of,)

IT Fluorination

(electrochem., of partially fluorinated enamines)

IT 7782-41-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination, electrochem., of partially fluorinated enamines)

IT 151630-21-6P 151630-22-7P 151630-23-8P 151630-24-9P 151630-25-0P

151630-26-1P 151630-27-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and electrochem. fluorination of)

IT 151630-28-3P 151630-29-4P 151630-30-7P 151654-82-9P 151654-83-0P

151654-84-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 111-92-2, Dibutylamine 124-02-7, Diallylamine 142-84-7, Dipropylamine

RL: RCT (Reactant); RACT (Reactant or reagent)

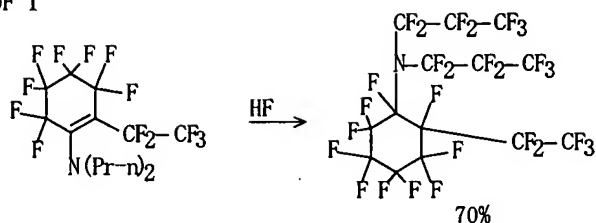
(reaction of, with perfluoroolefins)

IT 151630-31-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactions of, with secondary amines)

RX(1) OF 1



NOTE: electrochem.

L47 ANSWER 5 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 114:101067 CASREACT

TI Fluoroaliphatic esters of fluorosulfonic acid. 1. Reaction of higher fluoro olefins with electrochemically generated peroxydisulfonyl difluoride

AU Rogovik, V. M.; Koval'skii, Ya. I.; Delyagina, N. I.; Mysov, E. I.; Gida, V. M.; Grinberg, V. A.; Cherstkov, V. F.; Sterlin, S. R.; German, L. S.

CS Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR

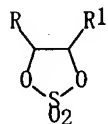
SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1990), (9), 2048-56

CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Russian

GI



AB Electrolysis of HSO_3F with RCF:CFR_1 [$\text{R} = (\text{CF}_3)_2\text{CF}$, $(\text{CF}_3)_3\text{C}$, C_2F_5 , C_3F_7 , $n\text{-C}_5\text{F}_{11}$, $\text{R}_1 = \text{CF}_3$; $\text{RR}_1 = (\text{CF}_2)_4$] in the presence of NaO_3SF gave 42.9-91.6% $\text{FSO}_3\text{CFRCFR}_1\text{O}_3\text{SF}$, along with $\leq 6.4\%$ $\text{RCOCR}_1\text{O}_3\text{SF-FSO}_3\text{CFRCOR}_1$, $\leq 3.5\%$ cyclic sulfates I, and/or 25.8-64.7% mixed isomeric dimeric bis(fluorosulfonates). $(\text{CF}_3)_2\text{C:CFC}_2\text{F}_5$ reacted analogously to 99.5% $\text{FSO}_3\text{C}(\text{CF}_3)_2\text{CF}(\text{O}_3\text{SF})\text{C}_2\text{F}_5$. ^{19}F NMR and mass-spectral data are given for most products.

CC 23-12 (Aliphatic Compounds)

ST addn peroxydisulfonyl fluoride perfluoro alkene; fluorosulfonate perfluoroaliph prepn NMR mass spectra

IT Addition reaction

(of electrochem. generated peroxydifluorosulfonyl fluoride with higher perfluoroalkenes)

IT Mass spectra

(of perfluoroaliph. fluorosulfonates)

IT Nuclear magnetic resonance

(of perfluoroaliph. fluorosulfonates, fluorine-19)

IT Perfluorocarbons

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkenyl, higher, addition reaction of, with electrochem. generated peroxydisulfonyl difluoride)

IT Compound (C10F22O6S2), m. 55-56°

Compound (C12F26O6S2), m. 90-92°

Compound (C16F34O6S2), m. 103-105°

RL: SPN (Synthetic preparation); PREP (Preparation)

IT 13709-32-5, Peroxydisulfonyl difluoride

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition reaction of electrochem. generated, with higher perfluoroalkenes)

IT 1584-00-5 1584-03-8 2070-70-4 65500-50-7 72487-69-5 72804-49-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with electrochem. generated peroxydisulfuryl difluoride)

IT 7782-41-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(nuclear magnetic resonance, of perfluoroaliph. fluorosulfonates, fluorine-19)

IT 355-75-9P 71917-17-4P 71917-18-5P 71917-19-6P 71917-21-0P
71917-22-1P 71917-23-2P 75677-97-3P 75688-00-5P 128478-72-8P
132182-97-9P 132182-98-0P 132182-99-1P 132183-01-8P 132183-02-9P
132183-03-0P 132183-04-1P 132183-05-2P 132183-06-3P 132209-47-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mass spectrum of)

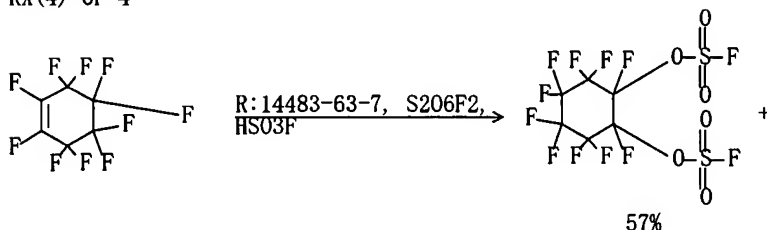
IT 75677-98-4P 132182-84-4P 132182-85-5P 132182-89-9P 132183-07-4P
132209-46-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

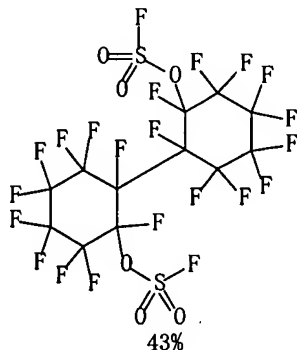
IT 132182-90-2P 132182-93-5P 132183-00-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, fluorine-19 NMR, and mass spectrum of)

RX(4) OF 4



RX(4) OF 4



NOTE: electrochem.

L47 ANSWER 6 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 114:41671 CASREACT

TI Fluorination of polyhalogenated unsaturated compounds with vanadium pentafluoride

AU Bardin, V. V.; Avramenko, A. A.; Furin, G. G.; Krasilnikov, V. A.; Karelin, A. I.; Tushin, P. P.; Petrov, V. A.

CS Inst. Org. Chem., Novosibirsk, 630090, USSR

SO Journal of Fluorine Chemistry (1990), 49(3), 385-400

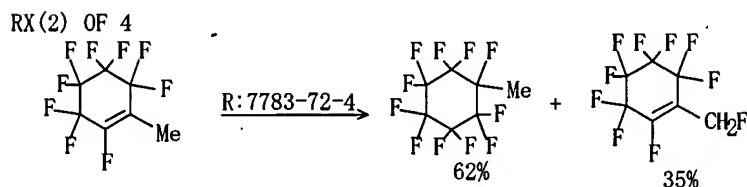
CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

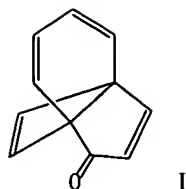
LA English

AB VF55 reacts with polyfluorinated and polychlorinated olefins, alkadienes, cycloalkenes and cyclodienes in CFC13 or without a solvent at -25° to 100°, forming products of addition of two fluorine atoms across the C:C bond. Thus, treating CF2:CFR [R = (CF2)4CFC1CF2C1] with VF5 gave 83% CF3CF2R with 100% alkene conversion.

CC 21-2 (General Organic Chemistry)
 ST fluorination polyfluoroalkene polyfluorocycloalkene polyfluoroarene;
 vanadium pentafluoride fluorination unsatd compd; alkane polyhalo;
 cycloalkane polyhalo; arene polyhalo; alkene polyhalo fluorination;
 cycloalkene polyhalo fluorination; cycloalkadiene polyhalo fluorination
 IT Fluorination
 (of polyhalogenated unsatd. compds. with vanadium pentafluoride)
 IT Alkenes, reactions
 Cycloalkenes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (halo, fluorination of)
 IT Alkyl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (unsatd., fluorination of)
 IT 7783-72-4, Vanadium pentafluoride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination by, of polyhalogenated unsatd. compds.)
 IT 87-68-3 127-18-4, reactions 303-04-8 336-19-6 377-70-8 392-42-7
 647-53-0 697-11-0 706-79-6 773-53-5 775-51-9 830-23-9
 1187-93-5 1584-03-8 2070-70-4 5492-89-7 5953-44-6 5954-49-4
 15145-21-8 28750-05-2 31665-17-5 31673-21-9 54939-04-7
 57113-75-4 67899-41-6 70695-62-4 111302-02-4 111302-04-6
 131045-00-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination of)
 IT 7782-41-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination, of polyhalogenated unsatd. compds. with vanadium
 pentafluoride)
 IT 76-12-0P 115-25-3P 335-47-7P 336-13-0P 336-14-1P 336-15-2P
 355-04-4P 355-20-4P 355-75-9P 375-35-9P 375-43-9P 432-16-6P
 665-16-7P 777-97-9P 1428-38-2P 2342-07-6P 2358-31-8P 10575-60-7P
 13772-77-5P 54326-26-0P 91374-74-2P 111180-52-0P 111302-03-5P
 111331-31-8P 111331-32-9P 111948-62-0P 111948-64-2P 120345-76-8P
 120345-77-9P 131044-87-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)



L47 ANSWER 7 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 112:118312 CASREACT
 TI Synthesis and photochemical reaction of [4.3.2]propella-2,4,8,10-tetraen-7-one
 AU Ohkita, Masakazu; Tsuji, Takashi; Suzuki, Masayuki; Murakami, Masashi;
 Nishida, Shinya
 CS Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan
 SO Journal of Organic Chemistry (1990), 55(5), 1506-13
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI



AB [4.3.2]Propella-2,4,8,10-tetraen-7-one (I) is synthesized from dihydroindanone in 4 steps in 10% overall yield. The electronic absorption spectrum of I suggests weak interactions among its π bonds, possibly longicyclic in mode. Direct photolysis of I leads to the formation of tricyclo[4.3.2.0_{1,4}]undeca-2,4,8,10-tetraen-7-one (II) and 6,7-benzobicyclo[3.2.0]hepta-3,6-dien-2-one (III) in aprotic solvents, presumably from its singlet excited state. The former product reverts to I upon irradiation. In MeOH the interconversion between I and II is partially quenched and a labile MeOH adduct, Me 2-tricyclo[5.2.0.0_{1,3}]nona-4,6,8-trieneacetate (IV) is produced from both I and II. The transformation of I into IV proceeds stereospecifically to give endo-IV at low temperature, which equilibrates with exo-IV at room temperature, presumably via a cyclobutadiene intermediate, Me 6-bicyclo[5.2.0]nona-1(7),2,4,8-tetraeneacetate (V) ($\Delta G_{\text{thermod.}} < 22 \text{ kcal/mol}$). IV undergoes only polymerization, possibly via V in solution at ambient temperature but rearranges to Me 1-indeneacetate under GLC conditions above 150.

CC 24-8 (Alicyclic Compounds)

ST propellatetraenone prepn photolysis; photochem reaction propellatetraenone

IT Photolysis

(of propellatetraenone)

IT 83-33-0P, 1-Indanone 24040-30-0P 124944-29-2P 124944-31-6P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, by photolysis of propellatetraenone)

IT 124944-30-5P

RL: PREP (Preparation)

(formation, NMR, and thermal equilibrium of, with indole isomer)

IT 75781-80-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(photochem. cycloaddn. reaction of, with dichloroethylene)

IT 156-60-5, trans-1,2-Dichloroethylene

RL: RCT (Reactant); RACT (Reactant or reagent)

(photochem. cycloaddn. reaction of, with dihydroindanone)

IT 125074-72-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and acetalization of, with ethylene glycol)

IT 124944-22-5P 124944-37-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and bromination of)

IT 124944-34-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and dehydration of)

IT 124944-23-6P 124944-25-8P 124944-38-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and dehydrobromination of)

IT 124944-27-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and desulfonylation of, with tri-Et phosphite)

IT 124991-93-1P 125074-71-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and hydride reduction of)

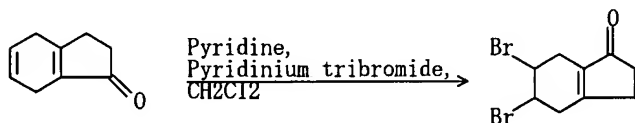
IT 124944-35-0P 124944-36-1P 125073-18-9P 125073-19-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

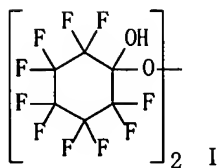
(Reactant or reagent)

- (preparation and oxidation of)
- IT 124944-24-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. cycloaddn. reaction of, with acetylene)
- IT 124944-21-4P, 3a, 7a-Ethano-1H-inden-1-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photochem. reactions of)
- IT 124944-32-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photolysis of, in methanol)
- IT 124991-94-2P 124991-95-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive dechlorination of)
- IT 124944-28-1P, 3a, 7a-Ethano-1H-inden-1-one 124944-33-8P 125073-17-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 124944-26-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, photolysis, and phenylthiolation of)

RX(8) OF 296



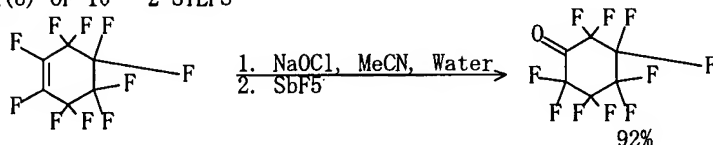
- L47 ANSWER 8 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
- AN 111:232124 CASREACT
- TI Synthesis and crystal structure of α, α' -dihydroxybis(perfluorocyclohexyl) peroxide
- AU Aleksandrov, A. V.; Kosnikov, A. Yu.; Antonovskii, V. L.; Lindeman, S. V.; Struchkov, Yu. T.; Gushchin, V. V.; Starostin, E. K.; Nikishin, G. I.
- CS Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR
- SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1989), (4), 918-23
CODEN: IASKA6; ISSN: 0002-3353
- DT Journal
- LA Russian
- GI



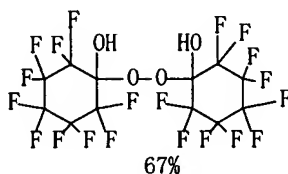
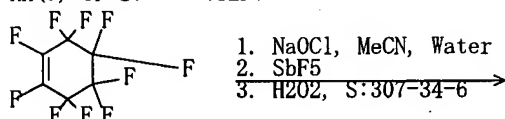
- AB The crystal structure of the title compound I (as its monohydrate), prepared in the reaction of stoichiometric quantities of perfluorocyclohexanone with 98% H₂O₂, was reported.
- CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 75
- ST perfluorocyclohexanone reaction hydrogen peroxide; peroxide
dihydroxybis(perfluorocyclohexyl) crystal mol structure; cyclohexyl peroxide
dihydroxyperfluoro

- IT Crystal structure
Molecular structure
(of dihydroxybis(perfluorocyclohexyl) peroxide)
- IT 6588-63-2
RL: PROC (Process)
(conversion of, to perfluorocyclohexene)
- IT 5927-67-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to perfluorocyclohexanone)
- IT 123762-54-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
- IT 355-75-9P, Perfluorocyclohexene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and epoxidn. of)
- IT 106813-73-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
- IT 1898-91-5P, Perfluorocyclohexanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with hydrogen peroxide)

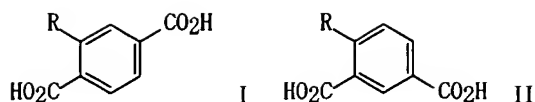
RX(6) OF 10 - 2 STEPS



RX(9) OF 10 - 3 STEPS

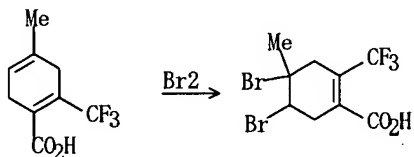


L47 ANSWER 9 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
AN 111:153303 CASREACT
TI A one-pot synthesis of polyfluoroalkyl-substituted tere- and isophthalic acids from polyfluoro-2-alkynoic acids
AU Yamanaka, Hiroki; Murakami, Akira; Kuwabara, Masaki; Fukunishi, Koushi; Nomura, Mototeru
CS Fac. Eng. Des., Kyoto Inst. Technol., Kyoto, 606, Japan
SO Chemistry Express (1989), 4(1), 21-4
CODEN: CHEXEU; ISSN: 0911-9566
DT Journal
LA English
GI

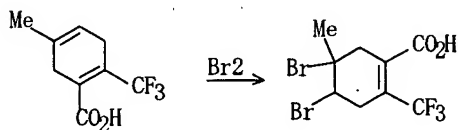


- AB Tere- and isophthalic acids I and II [R = CF₃, CHF₂, H(CF₂)₃, H(CF₂)₅] were prepared in one-pot from RC. tpbond. CO₂H and H₂C:CMech:CH₂ by sequential Diels-Alder reaction, bromination, dehydrobromination, and oxidation
- CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
- ST terephthalic acid fluoroalkyl; isophthalic acid fluoroalkyl; fluoroalkylterephthalic acid; fluoroalkylisophthalic acid
- IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Diels-Alder reaction of, with fluoroalkynoic acids)
- IT 110680-65-4 110680-66-5 110680-67-6 120801-99-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Diels-Alder reaction of, with methylbutadiene)
- IT 1483-46-1P 1483-47-2P 120985-72-0P 120985-73-1P 120985-74-2P
 120985-75-3P 122918-55-2P 122918-56-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

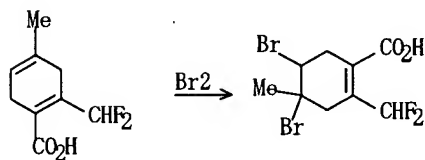
RX(9) OF 32



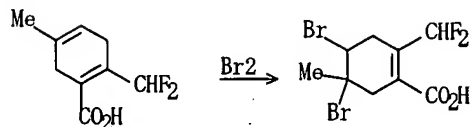
RX(10) OF 32



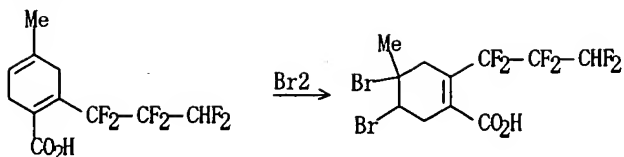
RX(11) OF 32



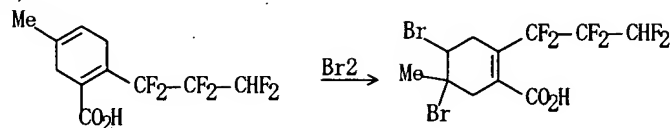
RX(12) OF 32



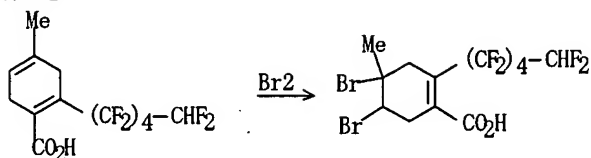
RX(13) OF 32



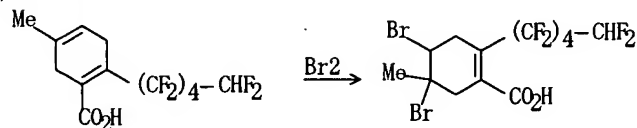
RX(14) OF 32



RX(15) OF 32



RX(16) OF 32



L47 ANSWER 10 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 111:7007 CASREACT

TI Synthesis of terephthalic acids containing polyfluoroalkyl groups

AU Kuwabara, Masaki; Murakami, Akira; Fukunishi, Koushi; Nomura, Mototeru; Yamanaka, Hiroki

CS Fac. Eng. Des., Kyoto Inst. Technol., Kyoto, 606, Japan

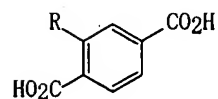
SO Journal of Fluorine Chemistry (1989), 42(1), 105-18

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

GI



I

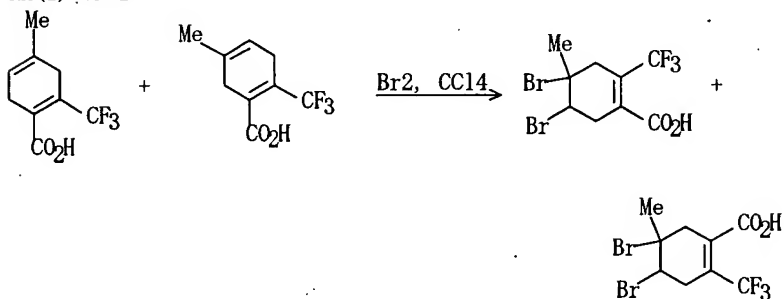
AB The syntheses of new terephthalic acids [I; R = CF₃, CHF₂, (CF₂)₂CHF₂, (CF₂)₄CHF₂] are described. These compds. were obtained by aromatization (bromination and dehydrobromination) of Diels-Alder adducts of polyfluoro-2-alkynoic acids with 2-methyl-1,3-butadiene, followed by oxidation with KMnO₄.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST terephthalic acid fluoroalkyl; Diels Alder adduct aromatization

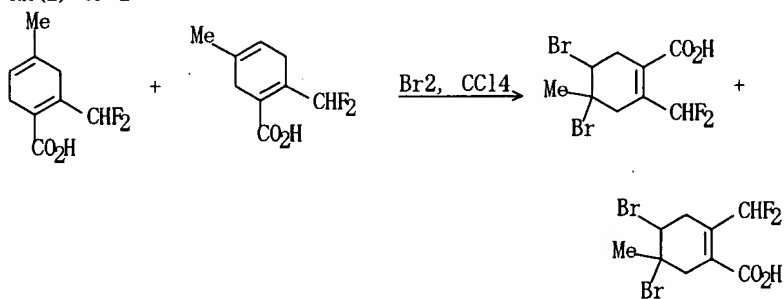
- IT Aromatization
(of Diels-Alder adducts of fluoroalkynoic acids and isoprene,
terephthalic acids from)
- IT 120802-01-9 120802-02-0 120802-03-1 120802-04-2 120802-05-3
120802-06-4 120802-07-5 120802-08-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)
- IT 120985-56-0 120985-57-1 120985-58-2 120985-59-3 120985-60-6
120985-61-7 120985-62-8 120985-63-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrobromination of)
- IT 120985-64-0 120985-65-1 120985-66-2 120985-67-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of)
- IT 120985-69-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and oxidation of)
- IT 1483-47-2P 120985-68-4P 120985-70-8P 120985-71-9P 120985-72-0P
120985-73-1P 120985-74-2P 120985-75-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RX(1) OF 27



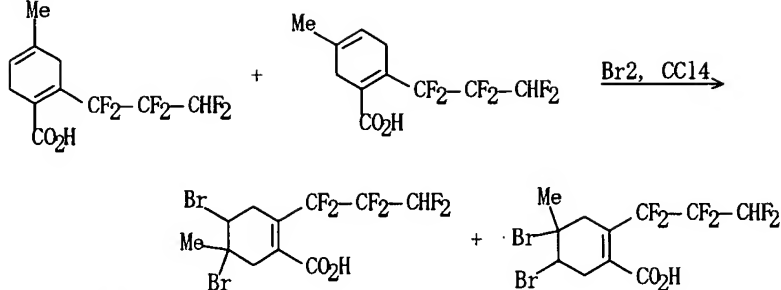
NOTE: 80% overall

RX(2) OF 27



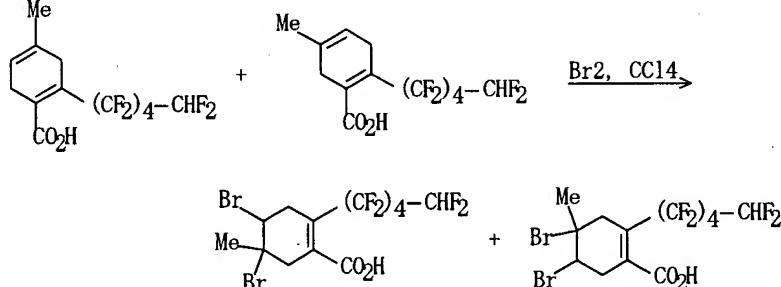
NOTE: 85% overall

RX(3) OF 27



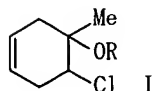
NOTE: 83% overall

RX(4) OF 27



NOTE: 80% overall

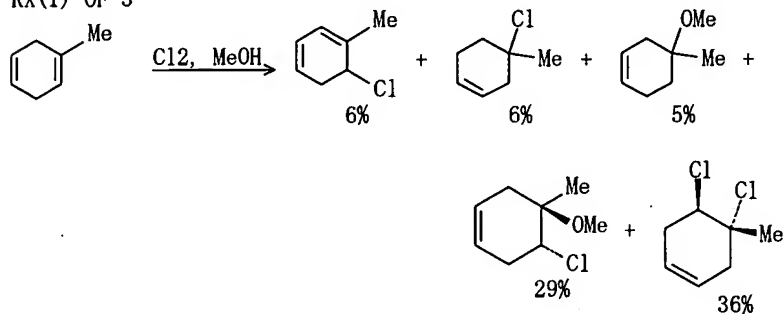
L47 ANSWER 11 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 110:114337 CASREACT
 TI Three component reactions. XVIII. Alkoxy- and acyloxychlorination of 1-methylcyclohexa-1,4-diene
 AU Beger, Joerg; Vogel, Titus
 CS Sekt. Chem., Bergakad. Freiberg, Freiberg, DDR-9200, Ger. Dem. Rep.
 SO Zeitschrift fuer Chemie (1988), 28(8), 289-90
 CODEN: ZECEAL; ISSN: 0044-2402
 DT Journal
 LA German
 GI



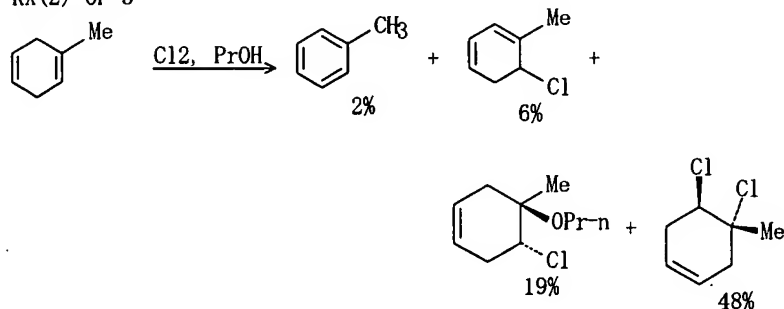
AB The title reaction gave 35.6-48.4% trans-4,5-dichloro-4-methylcyclohex-1-ene and 14.4-29.4% alkoxy-cyclohexenes I ($\text{R} = \text{Me}, \text{Pr}, \text{Ac}$) together with 6-15.8% 5-chloro-4-methylcyclohexa-1,3-diene. 4-Chloro-4-methylcyclohex-1-ene was obtained in 17.7% yield from the reaction with AcOH .
 CC 24-5 (Alicyclic Compounds)
 ST methylcyclohexadiene alkoxychlorination acyloxychlorination; chlorination alkoxylation acyloxylation methylcyclohexadiene
 IT Chlorination
 (alkoxylation or acyloxylation and, of methylcyclohexadiene)
 IT Alkoxylation
 (chlorination and, of methylcyclohexadiene)

IT 4313-57-9, 1-Methylcyclohexa-1,4-diene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (alkoxychlorination and acyloxychlorination of)
 IT 108-88-3P, preparation 119449-03-5P 119449-04-6P 119449-05-7P
 119449-06-8P 119449-07-9P 119449-08-0P 119449-09-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

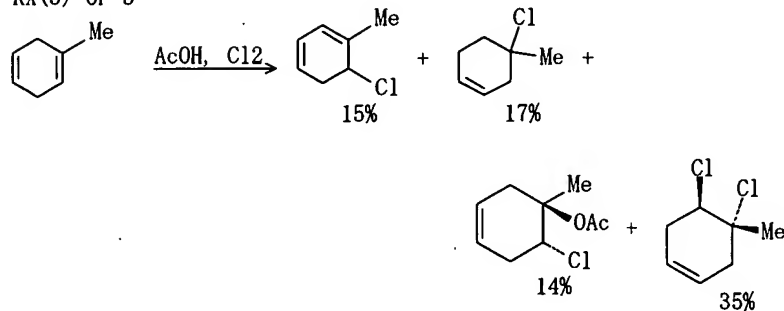
RX(1) OF 3



RX(2) OF 3

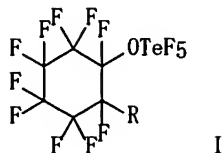


RX(3) OF 3



L47 ANSWER 12 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 109:148855 CASREACT
 TI Pentafluorotellurium oxide derivatives of fluorocarbons
 AU Schack, Carl J.; Christe, Karl O.
 CS Rocketdyne Div., Rockwell Int., Canoga Park, CA, 91304, USA
 SO Journal of Fluorine Chemistry (1988), 39(2), 153-62
 CODEN: JFLCAR; ISSN: 0022-1139
 DT Journal

LA English
GI



AB The reaction of xenon bis(pentafluorotellurium oxide), $\text{Xe}(\text{OTeF}_5)_2$, with excess perfluorobutadiene gives almost exclusively $\text{TeF}_5\text{OCF}_2\text{CF}:\text{CFCF}_2\text{OTeF}_5$ and only very little $\text{TeF}_5\text{OCF}_2\text{CF}(\text{OTeF}_5)\text{CF}:\text{CF}_2$, the first examples of TeF_5 -substituted unsatd. fluorocarbons. A similar reaction of perfluorocyclohexene produces, depending on the reaction temperature, exclusively the addition product I ($\text{R} = \text{OTeF}_5$), or predominantly the mixed addition, fluorination product I ($\text{R} = \text{F}$). In the case of TeF_5OF , an ambient temperature reaction with perfluorobenzene results, depending on the stoichiometry of the reaction, in the addition of either 1 or 2 mols. of TeF_5OF accompanied by the oxygenation of the ring to give a cyclohexanone derivative

CC 23-13 (Aliphatic Compounds)

Section cross-reference(s): 24

ST xenon bispentafluorotellurium oxide addn perfluorobutadiene;
perfluorocyclohexene addn xenon bispentafluorotellurium oxide; telluration
hexafluorobenzene fluoroxypentafluorotellurium

IT Addition reaction

(of pentafluorotellurium oxide to perfluorocarbons)

IT 392-56-3, Hexafluorobenzene 116486-95-4 116486-96-5 116486-97-6
116486-98-7 116486-99-8 116487-00-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition and fluorination reactions of, with
fluoroxypentafluorotellurium)

IT 83314-21-0, Fluoroxypentafluorotellurium

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition and fluorination reactions of, with hexafluorobenzene)

IT 25005-56-5, Xenon bis(pentafluorotellurium oxide)

RL: RCT (Reactant); RACT (Reactant or reagent)

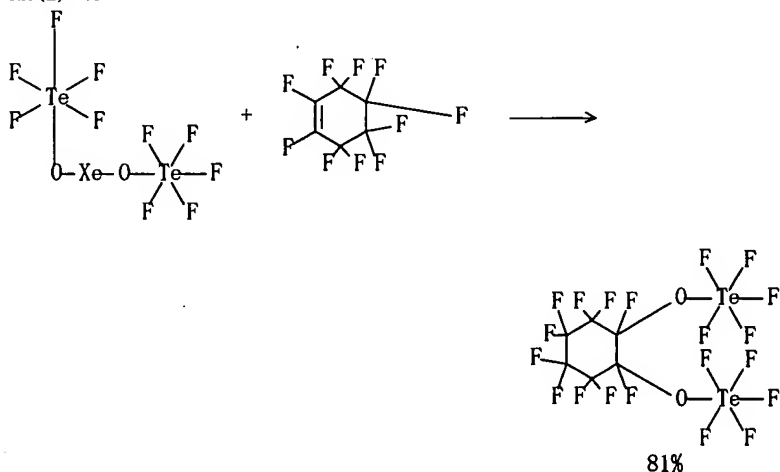
(addition reaction of, with perfluorobutadiene and perfluorocyclohexene)

IT 355-75-9, Perfluorocyclohexene 685-63-2, Hexafluoro-1,3-butadiene

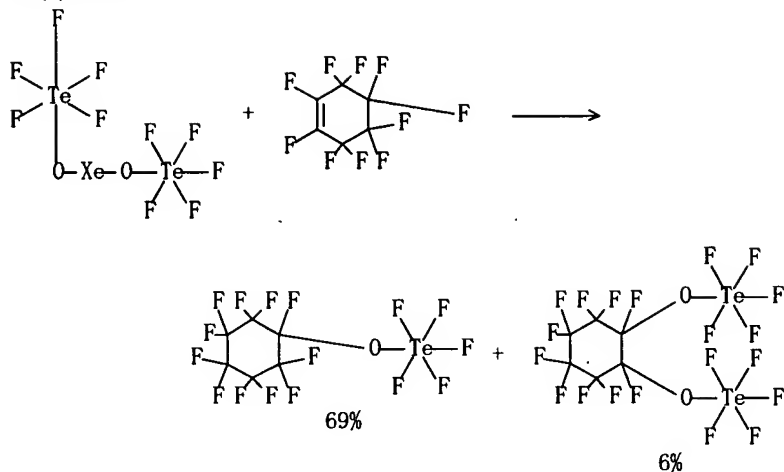
RL: RCT (Reactant); RACT (Reactant or reagent)

(addition reaction of, with xenon bis(pentafluorotellurium oxide))

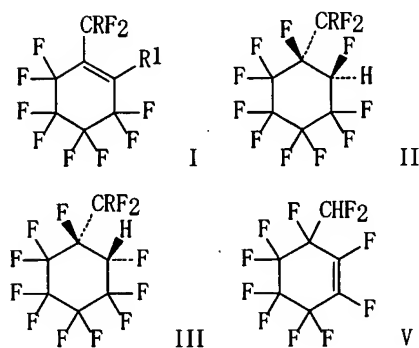
RX(2) OF 5



RX(3) OF 5



L47 ANSWER 13 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 109:92318 CASREACT
 TI Fluorocyclohexanes. Part XVII. Dehydrofluorination of the cis and trans isomers of 2H-1-(difluoromethyl)decafluorocyclohexane
 AU Bailey, John; Plevy, Raymond G.; Tatlow, John Colin
 CS Chem. Dep., Univ. Birmingham, Birmingham, B15 2TT, UK
 SO Journal of Fluorine Chemistry (1988), 39(2), 227-33
 CODEN: JFLCAR; ISSN: 0022-1139
 DT Journal
 LA English
 GI



AB Cyclohexene I ($\text{R} = \text{R}_1 = \text{H}$) was passed over CoF_3 at 165° to give the trifluoromethyl derivative I ($\text{R} = \text{F}$, $\text{R}_1 = \text{H}$) and cis- and trans-decafluorocyclohexanes, II and III ($\text{R} = \text{H}$, F). Dehydrofluorination of II ($\text{R} = \text{H}$) with aqueous KOH gave only nonafluorocyclohexene I ($\text{R} = \text{H}$, $\text{R}_1 = \text{F}$) (IV). In a slower reaction, dehydrofluorination of III ($\text{R} = \text{H}$) gave a 2:1 mixture of IV and cyclohexene V.
 CC 24-5 (Alicyclic Compounds)
 ST octafluorocyclohexene difluoromethyl fluorination; fluorination difluoromethyloctafluorocyclohexene; dehydrofluorination difluoromethyldecafluorocyclohexane; decafluorocyclohexane difluoromethyl dehydrofluorination; nonafluorocyclohexene difluoromethyl
 IT Dehydrofluorination
 (of (difluoromethyl)decafluorocyclohexanes by potassium hydroxide, (difluoromethyl)nonafluorocyclohexenes from)
 IT 7664-39-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrofluorination, of (difluoromethyl)decafluorocyclohexanes by
potassium hydroxide, (difluoromethyl)nonafluorocyclohexenes from)

IT 115880-31-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(gas phase fluorination of)

IT 115880-32-5P 115880-33-6P

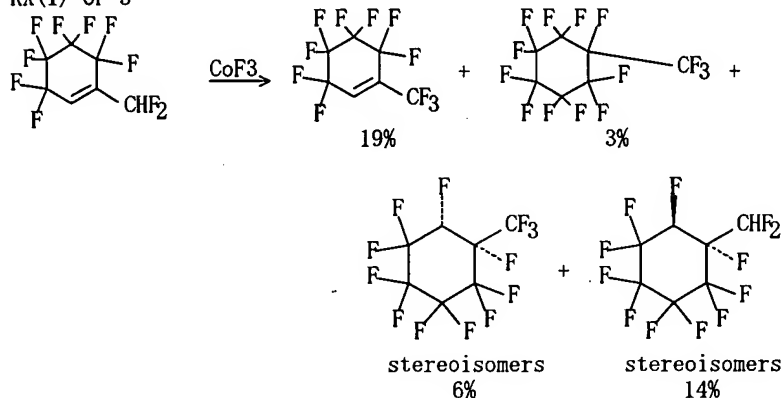
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and dehydrofluorination of)

IT 355-02-2P, Perfluoromethylcyclohexane 10534-43-7P 16804-81-2P

85359-76-8P 85359-78-0P 115880-34-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RX(1) OF 5



NOTE: gas phase

L47 ANSWER 14 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 108:21370 CASREACT

TI Reaction of polyfluoro cycloalkenes with vanadium, antimony, and niobium
pentafluorides

AU Bardin, V. V.; Avramenko, A. A.; Petrov, V. A.; Krasil'nikov, V. A.;
Karelin, A. I.; Tushin, P. P.; Furin, G. G.; Yakobson, G. G.

CS Novosib. Inst. Org. Khim., Novosibirsk, USSR

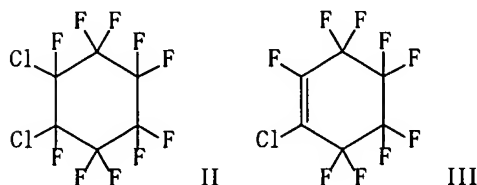
SO Zhurnal Organicheskoi Khimii (1987), 23(3), 593-7

CODEN: ZORKAE; ISSN: 0514-7492

DT Journal

LA Russian

GI



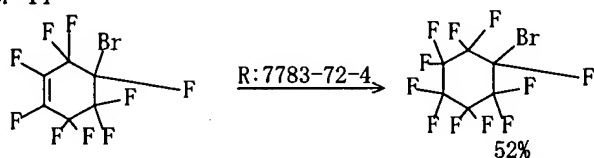
AB VF5 added F to polyfluorocycloalkenes to give the corresponding
cycloalkanes; e.g., hexafluorocyclobutene gave octafluorocyclobutane and
1,2-dichlorooctafluorocyclohexene (I) gave addition product II. With SbF5
fluorinolysis also occurred; e.g., I gave monochloro analog III. NbF5
failed to react.

CC 24-5 (Alicyclic Compounds)

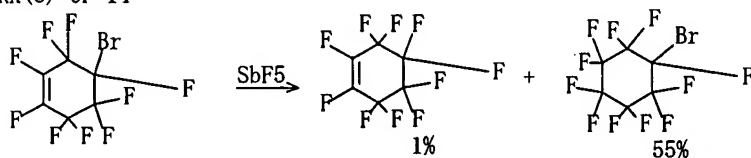
ST fluorocycloalkene antimony vanadium niobium pentafluoride; cycloalkene

- polyfluoro antimony vanadium niobium pentafluoride
- IT Addition reaction
(of polyfluorocycloalkenes with antimony or vanadium pentafluoride)
- IT Fluorination
(of polyfluorocycloalkenes, with antimony or vanadium pentafluoride)
- IT Cycloalkenes
RL: RCT (Reactant); RACT (Reactant or reagent)
(polyfluoro, fluorination of, with antimony or vanadium pentafluoride)
- IT 7783-68-8, Niobium pentafluoride
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted fluorination with, of dichlorooctafluorocyclohexene)
- IT 697-11-0, Hexafluorocyclobutene 706-79-6, 1-2-Dichlorohexafluorocyclopentene 5492-89-7 111948-63-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of, with vanadium pentafluoride)
- IT 7783-70-2, Antimony pentafluoride 7783-72-4, Vanadium pentafluoride
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination with, of polyfluorocycloalkenes)
- IT 7782-41-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination, of polyfluorocycloalkenes, with antimony or vanadium pentafluoride)
- IT 115-25-3P 336-13-0P, Bromoundecafluorocyclohexane 336-14-1P, 1,2-Dichlorodecafluorocyclohexane 336-15-2P, Chloroundecafluorocyclohexane 355-75-9P 2342-07-6P 2358-31-8P 10575-60-7P 28750-05-2P 91374-74-2P 111180-52-0P 111948-62-0P, cis-1,2-Dichlorooctafluorocyclopentane 111948-64-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 336-19-6, 1,2-Dichloro-octafluoro-cyclohexene 15145-21-8, 1-Chloro-nonafluoro-cyclohexane 57113-75-4, 4-Bromo-nonafluorocyclohexene
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of with antimony or vanadium pentafluoride)

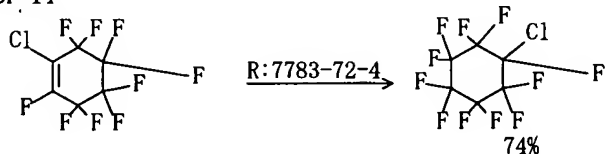
RX(2) OF 14



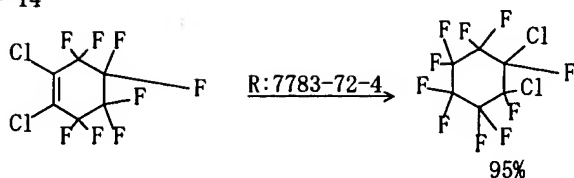
RX(3) OF 14



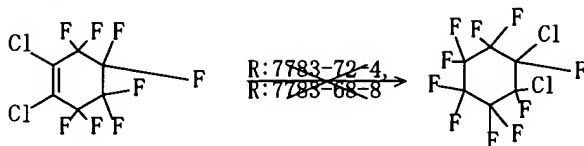
RX(4) OF 14



RX(6) OF 14

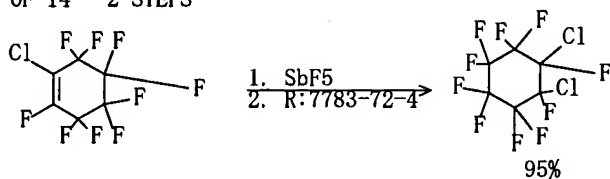


RX(11) OF 14

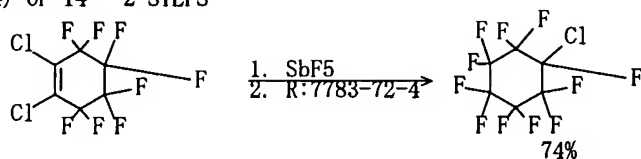


NOTE: failed reaction

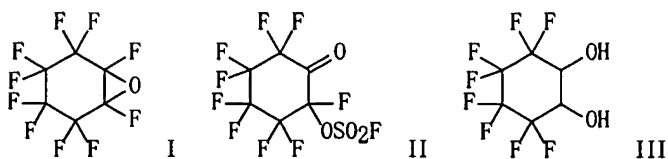
RX(13) OF 14 - 2 STEPS



RX(14) OF 14 - 2 STEPS

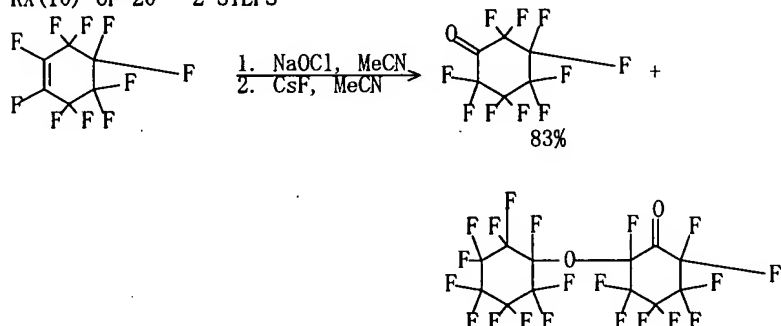


L47 ANSWER 15 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 107:236099 CASREACT
 TI Synthesis and properties of 1,2-epoxyperfluorocyclohexane
 AU Zapevalov, A. Ya.; Filyakova, T. I.; Peschanskii, N. V.; Kolenko, I. P.;
 Kodess, M. I.
 CS Inst. Khim., Sverdlovsk, USSR
 SO Zhurnal Organicheskoi Khimii (1986), 22(10), 2088-92
 CODEN: ZORKAE; ISSN: 0514-7492
 DT Journal
 LA Russian
 GI

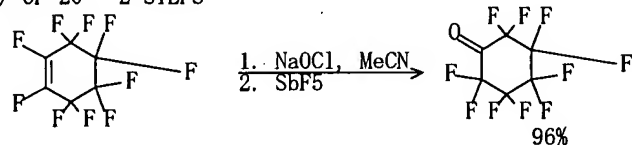


- AB The title compound I, prepared in 92% yield by epoxidn. of perfluorocyclhexene with NaOCl, was oxidized by CsF to give 83.6% perfluorocyclohexanone and an oligomeric perfluorinated ether ketone. Treating I with HS03F at 300° gave 37% cyclohexanone II which was reduced by LiAlH₄ to give 66% diol III. Addnl. obtained was 41.4% perfluoro-1,2-cyclohexanedione.
- CC 24-2 (Alicyclic Compounds)
- ST epoxyperfluorocyclohexane reaction; cyclohexane epoxy perfluoro; oxabicycloheptane perfluoro
- IT Epoxidation
(of perfluorocyclohexene with sodium hypochlorite, epoxyperfluorocyclohexane from)
- IT 355-75-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(epoxidn. of, by sodium hypochlorite)
- IT 5927-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
- IT 111511-41-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduction by lithium aluminum hydride)
- IT 1898-91-5P 83505-07-1P 111511-40-1P 111534-81-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 71917-20-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and reaction with cesium fluoride)

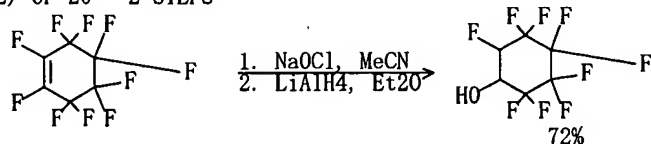
RX(10) OF 20 - 2 STEPS



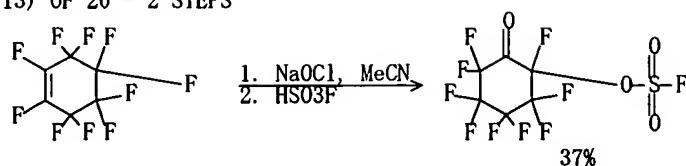
RX(11) OF 20 - 2 STEPS



RX(12) OF 20 - 2 STEPS



RX(13) OF 20 - 2 STEPS



L47 ANSWER 16 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 107:197566 CASREACT

TI Polyfluorocycloalkenes. Part XIX. Some reactions and compounds from 1,2-bis(trifluoromethyl)octafluorocyclohexene

AU Collins, David; Stephens, Robert; Tatlow, John Colin

CS Dep. Chem., Univ. Birmingham, Birmingham, B15 2TT, UK

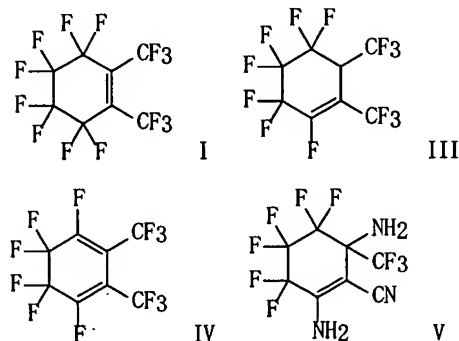
SO Journal of Fluorine Chemistry (1986), 32(2), 213-27

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

GI



AB Hydrogenation of the title compound (I) over Pd/C gave cis-bis(trifluoromethyl)octafluorocyclohexane (II) and a small amount of bis(trifluoromethyl)heptafluorocyclohexene III. Dehydrofluorination of II with aqueous KOH gave III and the bis(trifluoromethyl)hexafluorocyclohexadiene IV. Fluorination of IV with COF₃ also gave I. NH₃ reacted with I to give the diaminocyanocyclohexene V.

CC 24-5 (Alicyclic Compounds)

ST polyfluorocyclohexene; trifluoromethyloctafluorocyclohexene prepn
hydrogenation; amination trifluoromethyloctafluorocyclohexene;
fluorocycloalkene poly

IT 2995-00-8 3856-54-0 14100-80-2 14100-81-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrofluorination of)

IT 308-24-7, Undecafluorocyclohexane 355-75-9 374-79-8 777-97-9
110897-13-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(deuteration and dehydrofluorination of)

IT 306-98-9P 110897-07-9P 110897-08-0P 110897-11-5P 110897-12-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and dechlorination of)

IT 110897-10-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and dehydrofluorination of)

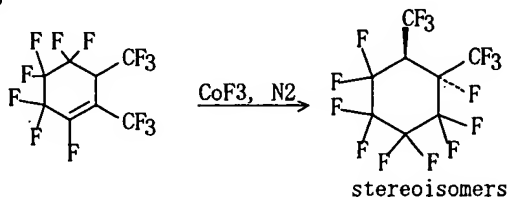
IT 110897-05-7P 110897-09-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

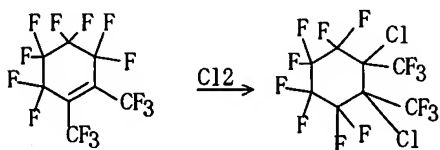
Search done by Noble Jarrell

- (preparation and fluorination of)
- IT 110897-06-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, fluorination, and dehydrofluorination of)
- IT 10534-39-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, hydrogenation, chlorination, and amination of)

RX(2) OF 46

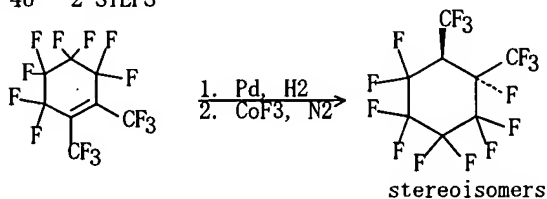


RX(4) OF 46

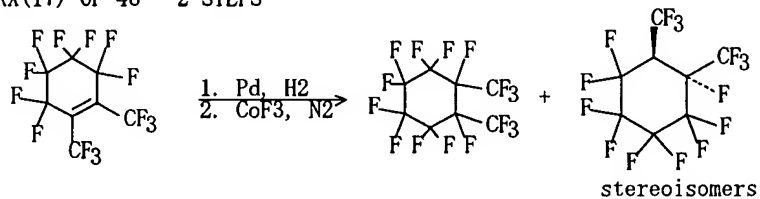


NOTE: photochem.

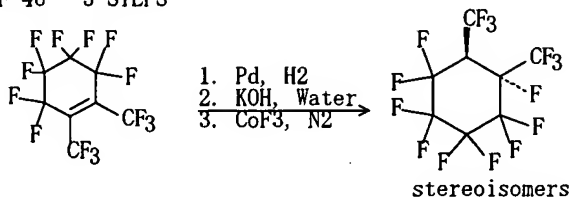
RX(14) OF 46 - 2 STEPS



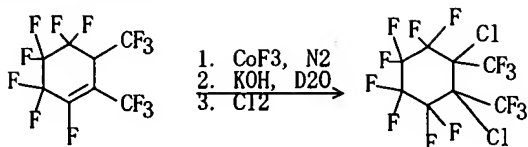
RX(17) OF 46 - 2 STEPS



RX(29) OF 46 - 3 STEPS



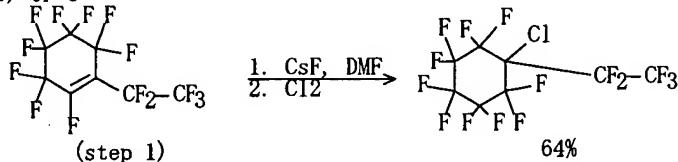
RX(30) OF 46 - 3 STEPS



NOTE: 3) photochem.

- L47 ANSWER 17 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 106:119170 CASREACT
 TI Stable cyclic perfluorinated carbanions and their NMR spectra
 AU Snegirev, V. F.; Delyagina, N. I.; Bakmutov, V. I.
 CS Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR
 SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1986), (6), 1325-31
 CODEN: IASKA6; ISSN: 0002-3353
 DT Journal
 LA Russian
 GI For diagram(s), see printed CA Issue.
 AB The reaction of perfluorocycloalkenes I ($n = 1$, $R = \text{C}_2\text{F}_5$; $n = 2$, $R = \text{CF}_3$; $n = 3$, $R = \text{C}_2\text{F}_5$) with CsF in DMF gave the carbanions (II), which reacted with Cl_2 to give the chloropolyfluoro compds. (III). The formation of II was followed by ^{13}C and ^{19}F NMR.
 CC 22-10 (Physical Organic Chemistry)
 ST cycloalkene perfluoro carbanion formation NMR; carbanion perfluorocycloalkane formation NMR; cycloalkane chloropolyfluoro
 IT Nuclear magnetic resonance
 (in perfluorinated alkylcyclohexenes and alkylcyclohexyl carbanions, of carbon-13 and fluorine-19)
 IT 106915-55-3P 106915-56-4P 106915-57-5P
 RL: PREP (Préparation)
 (formation, NMR and reaction with chlorine)
 IT 7782-41-4 14762-74-4
 RL: PRP (Properties)
 (nuclear magnetic resonance, in perfluorinated alkylcyclohexenes and alkylcyclohexyl carbanions, of carbon-13 and fluorine-19)
 IT 106915-58-6P 106915-59-7P 106915-60-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 780-87-0 61898-38-2 80308-96-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with fluoride, carbanion formation in)

RX(3) OF 3

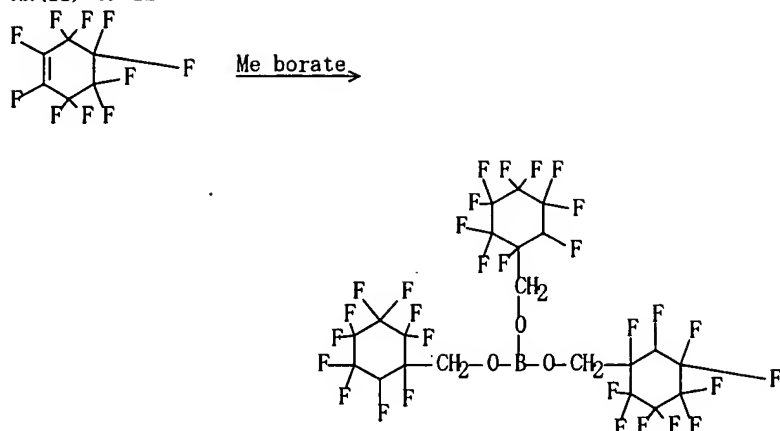


- L47 ANSWER 18 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 106:66698 CASREACT
 TI Free radical chemistry. Part 3. Substituent effects in additions of ethers to fluorinated alkenes
 AU Chambers, Richard D.; Grievson, Brian; Kelly, Noel M.
 CS Dep. Chem., Univ. Sci. Lab., Durham, DH1 3LE, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (11), 2209-13

CODEN: JCPRB4; ISSN: 0300-922X

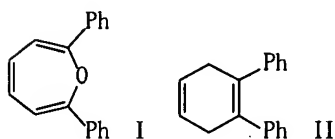
- DT Journal
 LA English
 AB Under γ -radiation (RCH₂)₂O (R = H, Me, Et, Pr) underwent addition reaction with CF₂:CFCF₃ to give varying amts. of RCHR10CH₂R, (RCHR1)₂O, and RCHR10CR1₂R (R1 = CF₂CHFCF₃). Steric effects on the competitive formation of these adducts are discussed. Captodative effects are not dominant in systems containing polyfluoroalkyl groups. Efficient free-radical addns. of trialkyl borates to fluorinated alkenes also occurred, but R₂CO₂Me (R₂ = Me, H, MeO, etc.) where less reactive.
- CC 23-3 (Aliphatic Compounds)
 Section cross-reference(s): 22
- ST addn hexafluoropropene ether; radical addn fluoro alkene ether; steric effect fluoroalkene addn ether; captodative effect fluoroalkene addn ether; substituent effect fluoroalkene addn ether; alkyl borate addn fluoro alkene; ester addn fluoro alkene
- IT Ethers, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with fluorinated alkenes)
- IT Addition reaction
 (of fluorinated alkenes with ethers, esters, and alkyl borates)
- IT Alkenes, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluoro, addition reaction of, with ethers, esters, and alkyl borates)
- IT Compound (C₂₁H₂₇BF₁₈O₃), b. 65-67° (0.5 mm Hg)
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- IT 116-15-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with ethers, esters, and alkyl borates in presence of γ -radiation or di-Bu peroxide)
- IT 79-20-9, Methyl acetate 107-31-3, Methyl formate 616-38-6, Dimethyl carbonate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with hexafluoropropene in presence of di-Bu peroxide)
- IT 60-29-7, Diethyl ether, reactions 111-43-3, Dipropyl ether 115-10-6, Dimethyl ether 142-96-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with hexafluoropropene in presence of γ -radiation)
- IT 121-43-7, Trimethyl borate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with polyfluoroalkenes in presence of γ -radiation)
- IT 355-75-9, Decafluorocyclohexene 559-40-0, Octafluorocyclopentene 697-11-0, Hexafluorocyclobutene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with tri-Me borate in presence of γ -radiation)
- IT 116-15-4DP, reaction products with tri-Bu borate 688-74-4DP, reaction products with hexafluoropropene
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)
- IT 382-31-0P 53005-38-2P 53005-39-3P 58705-93-4P 60417-68-7P 94412-75-6P 94412-76-7P 94412-78-9P 94412-80-3P 104725-00-0P 104725-01-1P 104725-02-2P 104764-60-5P 106538-74-3P 106538-75-4P 106538-76-5P 106538-77-6P 106538-78-7P 106538-79-8P 106538-80-1P 106538-81-2P 106538-82-3P 106549-82-0P 106549-83-1P 106549-84-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- IT 688-74-4, Tributyl borate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with hexafluoropropene in presence of γ -radiation)

RX(11) OF 12



NOTE: gamma radiation

L47 ANSWER 19 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 105:42617 CASREACT
 TI 2,7-Diphenyloxepin
 AU McManus, Michael J.; Berchtold, Glenn A.; Boyd, Derek R.; Kennedy, Deirdre A.; Malone, John
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1986), 51(14), 2784-7
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI

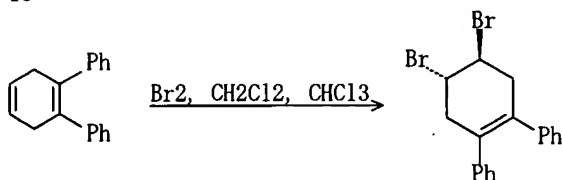


AB Diphenyloxepin I was prepared from the cyclohexadiene II in 3 steps. Acid-catalyzed isomerization of I gives 2,6-diphenylphenol in quant. yield. X-ray crystal structure anal. indicates that I exists in a boat conformation in the solid state.
 CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 75
 ST phenyloxepin prepn isomerization crystal structure; oxepin diphenyl isomerization
 IT Conformation and Conformers
 Crystal structure
 (of diphenyloxepin)
 IT Rearrangement
 (of diphenyloxepin, diphenylphenol from)
 IT 17351-29-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of)
 IT 20834-02-0 70238-90-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination-dehydrobromination of)
 IT 2432-11-3P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, by acid-catalyzed isomerization of diphenyloxepin)
 IT 102342-19-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)

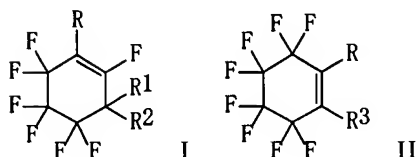
Search done by Noble Jarrell

- (preparation and dehydrobromination-ring cleavage of, diphenyloxepin from)
- IT 102367-83-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and epoxidn. of)
- IT 102342-18-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and isomerization and crystal structure of)
- IT 93654-94-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RX(1) OF 13



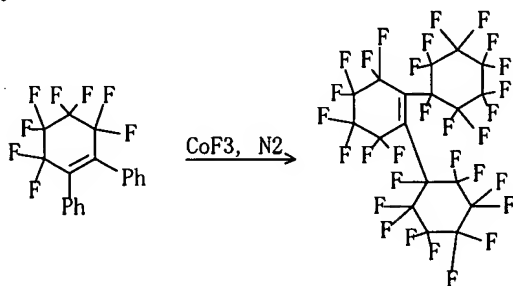
- L47 ANSWER 20 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
AN 104:206743 CASREACT
TI Polyfluorocycloalkenes. Part XVIII. Aryl adducts of decafluorocyclohexene
AU Coe, Paul L.; Oldfield, David; Tatlow, John Colin
CS Dep. Chem., Univ. Birmingham, Birmingham, B15 2TT, UK
SO Journal of Fluorine Chemistry (1985), 28(4), 453-60
CODEN: JFLCAR; ISSN: 0022-1139
DT Journal
LA English
GI



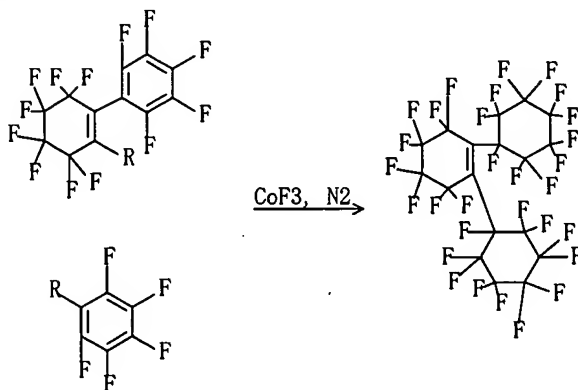
- AB Cyclohexene I (R-R2 = F) reacted with aniline to give I (R = PhNH, R1R2 = PhN), which was hydrolyzed by HCl to I (R1R2 = O). I (R-R2 = F) reacted with PhLi to give I (R = Ph) and II (R = R3 = Ph). The former product was attacked by C6F5Li at -40° C to give II (R = Ph, R3 = C6F5). PhLi reacted with II (R = R3 = C6F5) to give II (R = C6F5, R3 = p-PhC6F4) and II (R = R3 = p-PhC6F4); II (R = R3 = Ph, C6F5) were fluorinated by CoF3 to give II (R = R3 = undecafluorocyclohexyl).
- CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 25
- ST perfluorocyclohexene fluorophenyl; fluorination
pentafluorophenylcyclohexene; cyclohexene perfluoro
- IT 363-72-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with fluorocyclohexane derivative)
- IT 102118-87-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of)
- IT 102118-85-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

- (Reactant or reagent)
(preparation and hydrolysis of)
- IT 10575-65-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with phenyllithium and pentafluorophenyl
lithium)
- IT 102118-86-5P 102118-88-7P 102118-89-8P 102118-90-1P 102136-95-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 62-53-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with decafluorocyclohexene)
- IT 591-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with fluorocyclohexene derivs.)
- IT 5121-95-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenyllithium and fluorination of)
- IT 355-75-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with aniline and phenyllithium)

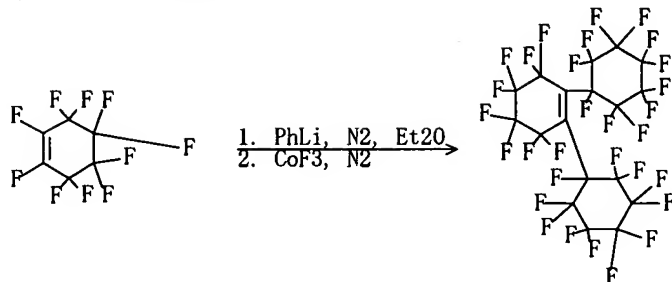
RX(4) OF 10



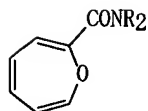
RX(7) OF 10



RX(10) OF 10 - 2 STEPS



L47 ANSWER 21 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 102:184659 CASREACT
 TI Aromatization of benzamide 1,2-oxide and N,N-dimethylbenzamide 1,2-oxide
 AU Busch, Frank R.; Berchtold, Glenn A.
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1985), 50(10), 1590-2
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI



I

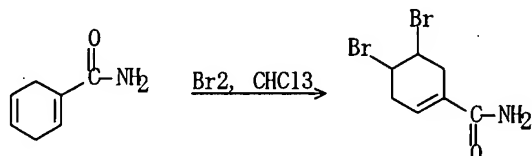
AB The mechanisms for aromatization of the title compds. I (R = H, Me) were examined through product studies and studies with the D-labeled analogs. Results from I (R = H) show that the relative amts. of C1-O and C2-O cleavage under acidic and neutral conditions are similar to those observed previously for the corresponding Me ester and carboxylic acid derivs. Aromatization of the cation derived from initial C2-O cleavage occurred by both substituent loss and substituent migration; substituent loss was the major pathway under acid-catalyzed conditions and the minor pathway under neutral conditions. Substantially more C1-O cleavage was observed with I (R = Me). For reaction proceeding via C2-O cleavage of I (R = Me), substituent loss predominated over substituent migration at pH 0.1, but only substituent migration was observed at higher pH (4.0, 7.0).

CC 22-13 (Physical Organic Chemistry)
 ST aromatization benzamide oxide mechanism
 IT Aromatization
 (of benzamide oxides, mechanism of)
 IT 108-31-6, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Diels-Alder reaction of, with benzamide oxides)
 IT 95673-76-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (amidation of)
 IT 95673-81-7P 95673-82-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and aromatization of, mechanism of)
 IT 95673-77-1P 95673-78-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and bromination of)

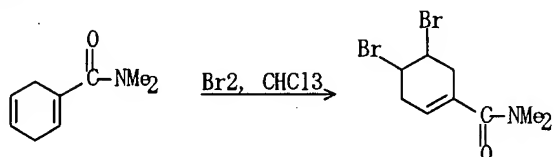
Search done by Noble Jarrell

- IT 95673-79-3P 95673-80-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and dehydrobromination of)
- IT 95673-83-9P 95673-84-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and epoxidn. of)
- IT 65-45-2P 1778-08-1P 95673-85-1P 95673-86-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

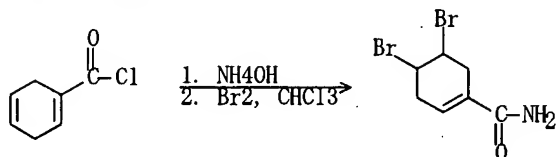
RX(3) OF 40



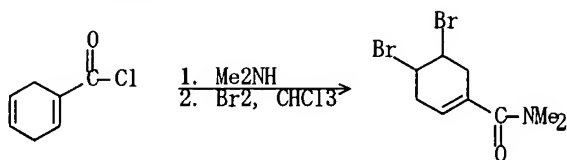
RX(4) OF 40



RX(13) OF 40 - 2 STEPS



RX(14) OF 40 - 2 STEPS

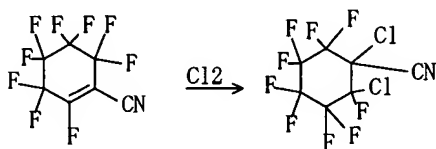


L47 ANSWER 22 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 101:6660 CASREACT
 TI Reactions of polyfluorocyclohexane- and polyfluorocyclohexenecarbonitriles
 AU Phull, Gurjeet S.; Plevy, Raymond G.; Tatlow, John Colin
 CS Dep. Chem., Univ. Birmingham, Birmingham, B15 2TT, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (3), 455-8
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 AB Gas-phase reaction of undecafluorocyclohexanecarbonitrile (RNC) (I) with CoF_3 or AgF_2 caused stepwise saturation of the C.tplbond.N bond to give RCF:NF

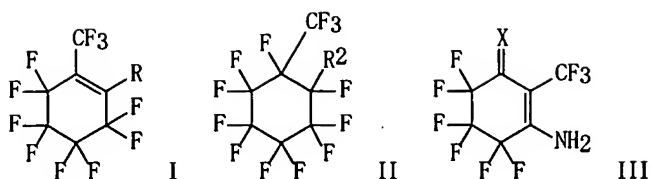
and RCF₂NF₂, whereas reaction in a sealed tube with AgF₂ or AgF gave (RCF₂N:)₂ and tris(undecafluorocyclohexyl)-s-triazine, resp. Treatment of I with aqueous R₁NHR₂ (R₁ = H, R₂ = Me, CHMe₂; R₁ = R₂ = Me) gave the corresponding RC(:NH)NR₁R₂. Vapor-phase fluorination of C₆F₅CN by CoF₃ or KCoF₄ gave I and nonafluorocyclohex-3-enecarbonitrile (II). Oxidation of II by KMnO₄ gave 3-cyanoheptafluorohexane-1,6-dioic acid. Nonafluorocyclohex-1-enecarbonitrile (III) underwent classical nucleophilic addition-elimination sequences with MeOH and with NaOMe to give methoxylated products, whereas reaction with NH₃ gave 2-aminohexafluoro-6-iminocyclohex-1-enecarbonitrile.

- CC 24-5 (Alicyclic Compounds)
 ST fluorocyclohexanecarbonitrile fluorination; fluorination
 perfluorocyclohexanecarbonitrile; addn alkyl amine
 perfluorocyclohexanecarbonitrile; fluorocyclohexylazomethane; azomethane
 bisperfluorocyclohexyl; fluorobenzonitrile fluorination;
 fluorocyclohexenecarbonitrile nucleophile substitution
 IT Amines, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with perfluorocyclohexanecarbonitrile)
 IT Fluorination
 (of perfluorocyclohexanecarbonitrile)
 IT 74-89-5, reactions 75-31-0, reactions 124-40-3, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with perfluorocyclohexanecarbonitrile)
 IT 51579-56-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination and amine addition reactions of)
 IT 773-82-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluorination of)
 IT 90408-42-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and oxidation of)
 IT 51685-11-1P 90408-36-9P 90408-37-0P 90408-38-1P 90408-39-2P
 90408-40-5P 90408-41-6P 90408-44-9P 90408-46-1P 90408-47-2P
 90408-48-3P 90408-49-4P 90408-50-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 90408-45-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactions of, with nucleophiles)

RX(13) OF 26



- L47 ANSWER 23 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 99:38076 CASREACT
 TI Polyfluorocycloalkenes. Part XVI. Some addition reactions of
 1-trifluoromethylnonafluorocyclohex-1-ene
 AU Carter, Paul A.; Patrick, Colin R.; Tatlow, John Colin
 CS Chem. Dep., Univ. Birmingham, Birmingham, B15 2TT, UK
 SO Journal of Fluorine Chemistry (1982), 21(4), 407-11
 CODEN: JFLCAR; ISSN: 0022-1139
 DT Journal
 LA English
 GI



AB Perfluoro(methylcyclohexene) (I, R = F) reacted with R_1OH ($R_1 = Me, Et$) to give I ($R = OR_1$). Fluorination of I ($R = OMe$) with CoF_3 gave II ($R_2 = OMe, OCH_2F, OCHF_2$). Oxidation of I ($R = OR_1$) gave $(HO_2CCF_2)_2CF_2$. I ($R = F$) and NH_3 formed enamine III ($X = NH$) which was hydrolyzed to III ($X = O$). I ($R = F$) was defluorinated by Fe at $440^\circ - 500^\circ$ to $C_6F_5CF_3$.

CC 24-5 (Alicyclic Compounds)

ST fluorocyclohexene oxidn defluorination fluorination; perfluorocyclohexene oxidn defluorination fluorination; cyclohexene fluoro oxidn defluorination fluorination

IT 1551-37-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 85577-99-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

IT 1696-31-7P 85578-00-3P 85578-01-4P 85578-02-5P 85578-03-6P

85578-04-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 424-33-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by oxidation of fluorinated cyclohexene derivs.)

IT 434-64-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from fluorinated cyclohexene derivative)

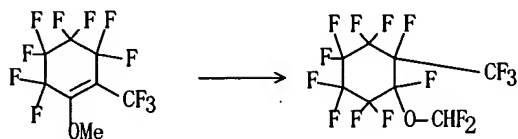
IT 85577-98-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, oxidation, and fluorination of)

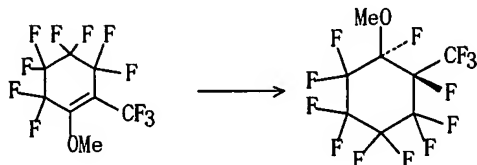
IT 432-16-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with alcs. or iron gauze)

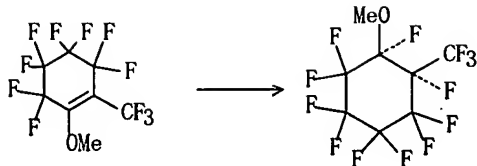
RX(2) OF 7



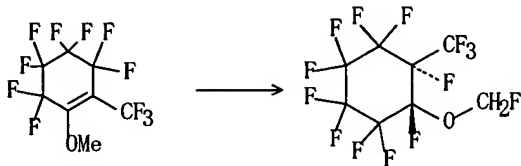
RX(3) OF 7



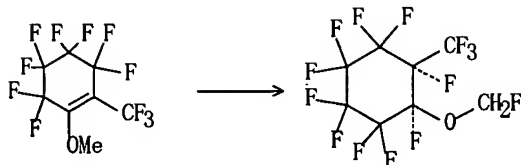
RX(4) OF 7



RX(5) OF 7



RX(6) OF 7



L47 ANSWER 24 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 98:106741 CASREACT

TI The preparation and properties of perfluoro-n-heptylbromine(V) tetrafluoride

AU Habibi, M. H.; Sams, L. C.

CS Dep. Chem., Texas Woman's Univ., Denton, TX, 76204, USA

SO Journal of Fluorine Chemistry (1982), 21(3), 287-93

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

AB F3C(CF2)6BrF4 (I) was prepared by fluorinating F3C(CF2)6Br with F, and characterized by IR, 19F-NMR, and mass spectra. 1,2-Dichlorohexafluorocyclopentene and 1,2-dichlorooctafluorocyclohexene were readily fluorinated by I.

CC 23-3 (Aliphatic Compounds)

Section cross-reference(s): 24

ST bromine tetrafluoro perfluoroheptyl; cyclopentane dichlorooctafluoro; cyclooctane dichlorotetradecafluoro; heptane bromoperfluoro fluorination; fluorination bromoperfluoroheptane; perfluoroheptylbromine tetrafluoride

fluorinating agent

IT Fluorination

(agents, perfluoroheptylbromine tetrafluoride)

IT 375-88-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination of)

IT 336-19-6 706-79-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorination of, by perfluoroheptylbromine tetrafluoride)

IT 84918-98-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and use of, as fluorinating agent)

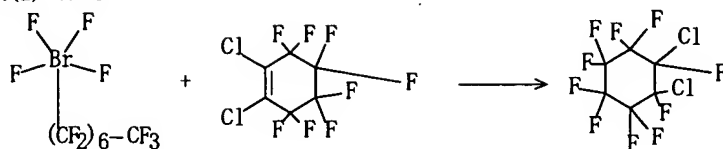
IT 376-75-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

Search done by Noble Jarrell

RX(2) OF 2



L47 ANSWER 25 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 97:92043 CASREACT

TI Polyfluoro-1,2-epoxyalkanes and -cycloalkanes. Part I. Preparation of some polyfluoro-1,2-epoxycyclohexanes

AU Coe, Paul L.; Mott, Andrew W.; Tatlow, John Colin

CS Chem. Dep., Univ. Birmingham, Birmingham, B15 2TT, UK

SO Journal of Fluorine Chemistry (1982), 20(2), 243-54

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA English

AB Polyfluorocyclohexenes with H, Br, and OMe substituents yielded the corresponding 1,2-epoxides when treated with aqueous NaOCl containing some MeCN. 4,5-Dibromooctafluoro-1,2-epoxycyclohexane was debrominated with Zn dust to give a mixture of octafluoro- and 4H-heptafluoro-1,2-epoxycyclohex-4-ene. Decafluoro- and 4,5-dibromooctafluoro-1,2-epoxycyclohexane gave with KF-MeCN, the corresponding K perhalocyclohexyl oxides; heating these gave the analogous cyclohexanones, and treatment with MeI the Me ethers. The unsatd. 1,2-epoxides also gave Me ethers on treatment with KF, followed by methylation.

CC 27-2 (Heterocyclic Compounds (One Hetero Atom))

ST polyfluorocycloalkene epoxidn; cycloalkene polyfluoro epoxidn

IT Epoxidation

(of polyfluorocycloalkenes)

IT 355-75-9 376-54-5 775-44-0 777-98-0 1428-38-2 6733-14-8

57113-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(epoxidn. of)

IT 377-70-8 775-51-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(oxidation of)

IT 82745-93-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and chlorination of)

IT 82745-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and debromination of)

IT 16621-89-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and decomposition of)

IT 82745-94-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and fluorination of)

IT 82745-98-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methylation of)

IT 82745-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with alkoxide)

IT 5927-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

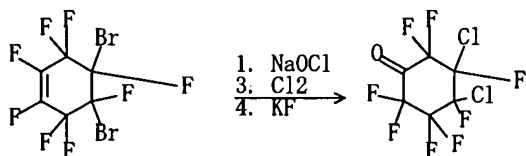
(Reactant or reagent)

(preparation and reaction of, with potassium fluoride)

IT 1898-91-5P 4943-08-2P 82745-87-7P 82745-88-8P 82745-89-9P
 82745-91-3P 82745-92-4P 82745-96-8P 82745-97-9P 82745-99-1P
 82746-00-7P 82746-01-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RX(25) OF 25 - 4 STEPS



L47 ANSWER 26 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 96:142974 CASREACT

TI Synthesis and conformational properties of 3,8-phosphonanedione 1-oxides

AU Quin, Louis D.; Middlemas, Eric D.; Rao, Nandakumar S.; Miller, Richard W.; McPhail, Andrew T.

CS Gross Chem. Lab., Duke Univ., Durham, NC, 27706, USA

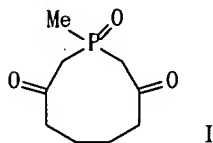
SO Journal of the American Chemical Society (1982), 104(7), 1893-900

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

GI



AB Ozonolysis at -78° of 3-phospholene derivs. with cyclohexane or substituted cyclohexanes fused at the double bond provides a useful route to derivs. of the 3,8-phosphonanedione 1-oxide system. Synthesized were the 1-Me (I), 1-Ph, 1-hydroxy, 1-phenyl-cis-5,6-dimethyl, 1-phenyl-trans-5,6-dibromo and 1-phenyl-5,6-epoxy derivs. Opening of the 9,10 bond of a phenanthrene fused to a 3-phospholene provided a dibenzod[f]phosphonanedione derivative I, shown by x-ray anal. to exist in a twist chair-chair form in the solid state, undergoes rapid interconversion of conformers at room temperature, giving an averaged ^{13}C NMR spectrum. The interconversion is halted at -97° , where signals for 2 conformers are obtained. 1-Phenyl-5,6-dibromo-3,8-phosphonanedione 1-oxide, which x-ray anal. also showed to be in a twist chair-chair form in the solid state, however, showed nonequivalence of comparable ring carbons, implying the existence of a strongly biased equilibrium or a high barrier to ring inversion. The dibenzod[f]phosphonanedione derivative has marked rigidity, and the ^{13}C NMR spectrum reveals that comparable ring carbons are nonequiv. at room temperature. The other phosphonanedione derivs. gave ^{13}C NMR spectra showing equivalence of comparable ring carbons, either through conformational interconversion or adoption of a sym. conformation.

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

ST phosphonanedione prepn crystal structure; dibenzophosphonanedione;
 ozonolysis phospholene; mol structure phosphonanedione; conformation
 phosphonanedione

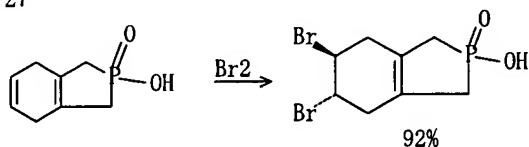
IT Conformation and Conformers

Crystal structure

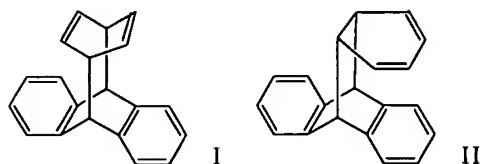
Molecular structure

- (of phosphonanedione oxides)
- IT 54290-41-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(McCormack cycloaddn. reaction of)
- IT 7789-60-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(adduct with diene)
- IT 80754-62-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn and reduction of)
- IT 65114-88-7P 75531-99-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
- IT 55781-96-9P 65114-89-8P 65482-10-2P 65482-11-3P 70179-63-4P
70179-64-5P 70179-65-6P 74078-07-2P 74078-08-3P 75401-33-1P
75401-34-2P 75401-35-3P 75401-36-4P 80461-86-5P 80754-56-9P
80754-58-1P 80754-59-2P 80754-60-5P 80754-61-6P 80754-63-8P
80794-93-0P 80794-94-1P 80794-95-2P 80794-96-3P 80794-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 1073-47-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diene)
- IT 676-83-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylenecyclohexane)
- IT 2819-48-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylphosphonous dichloride)
- IT 2548-47-2 80754-57-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylphosphonous dibromide)
- IT 33383-70-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tris(dimethylamino)phosphine)

RX(12) OF 27

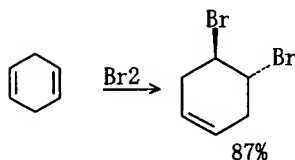


L47 ANSWER 27 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
AN 96:84904 CASREACT
TI Chemistry of exciplexes. 12. Chemistry of heterodimers of benzene and anthracene
AU Yang, Nien Chu C.; Chen, Ming Jang; Chen, Peter; Mak, Kwok Tim
CS Dep. Chem., Univ. Chicago, Chicago, IL, 60637, USA
SO Journal of the American Chemical Society (1982), 104(3), 853-5
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
GI



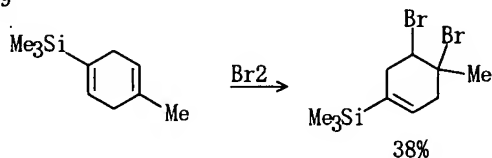
- AB Photocycloaddn. of substituted 1,3-cyclohexadienes to anthracene gave the $4\pi s + 4\pi s$ cycloadduct (I) and $4\pi s + 2\pi s$ cycloadduct (II) of benzene and anthracene in high purity (>99.8%). Thermal and photochem. cycloreversions to benzene and anthracene were observed for both adducts. Kinetic data clearly indicated that the thermal cycloreversion of I is a stepwise process, while that of II is concerted. Photolyses of both compds. at 0° yielded excited anthracene. The quantum yields of anthracene fluorescence, $\phi_f = 0.31$ for I and $\phi_f = 0.030$ for II, showed that the conversion of excited I to excited anthracene is a highly efficient process (80%), while that of excited II is much less efficient. The relation of these results to predictions made on orbital and state symmetry considerations was discussed.
- CC 22-8 (Physical Organic Chemistry)
- ST anthracene benzene cycloadduct cycloreversion; photochem cycloreversion anthracene benzene cycloadduct; fluorescence anthracene benzene cycloadduct photolysis; cycloaddn photochem anthracene cyclohexadiene deriv
- IT Fluorescence
(of anthracene from cycloreversion of anthracene-benzene cycloadducts)
- IT Kinetics of dissociation
(of anthracene-benzene cycloadducts)
- IT Cycloaddition reaction
(photochem., of anthracenes with cyclohexadienes)
- IT 592-57-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)
- IT 80409-72-9 80409-73-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloreversion of, kinetics of)
- IT 80409-74-1 80409-75-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn. reaction of, with anthracene)
- IT 120-12-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. cycloaddn. reaction of, with cyclohexadienes)
- IT 80446-29-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acetalization of)
- IT 80409-80-9P 80409-81-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrobromination of)
- IT 42846-36-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
- IT 80409-76-3P 80409-79-6P 80446-28-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with tert-butyllithium)
- IT 80409-78-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
- IT 80409-77-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RX(3) OF 5



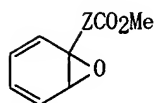
L47 ANSWER 28 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 94:208930 CASREACT
 TI Aromatization of arene 1,2-oxides. 1-(Trimethylsilyl)benzene 1,2-oxide
 AU Van Epp, James E., Jr.; Boyd, Derek R.; Berchtold, Glenn A.
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1981), 46(9), 1817-20
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 AB Aromatization of 1-(trimethylsilyl)benzene 1,2-oxide affords a mixture of o-(trimethylsilyl)phenol and phenol, the ratio of which is pH dependent. Aromatization of [5-2H]-1-(trimethylsilyl)benzene 1,2-oxide gave the following results. (1) At pH 1.1 or 7 all the deuterium label in o-(trimethylsilyl)phenol was para to the hydroxyl group. (2) At pH 1.1 the phenol formed was exclusively [4-2H]phenol, but at pH 7 it was 70-75% [4-2H]phenol and 25-30% [3-2H]phenol. The pathway of the aromatization reaction is discussed.
 CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25
 ST aromatization silylbenzene oxide; benzene silyl oxide aromatization; phenol trimethylsilyl; deuterium labeled phenol
 IT Aromatization
 (of trimethylsilylbenzene oxide)
 IT 69616-44-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aromatization of)
 IT 2060-89-1 3728-43-6 31825-45-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclohexadiene derivative from)
 IT 106-44-5P, preparation 108-39-4P, preparation 108-95-2P, preparation
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, from aromatization of benzene oxide)
 IT 76684-25-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and aromatization of)
 IT 108-95-2P, preparation 7329-50-2P 15288-53-6P 18036-83-4P
 54380-43-7P 55861-01-3P 55861-02-4P 69616-39-3P 69616-40-6P
 69616-41-7P 69616-43-9P 69616-45-1P 69616-46-2P 69616-51-9P
 76684-26-9P 76684-27-0P 76684-28-1P 76684-29-2P 76684-30-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 95-56-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chlorotrimethylsilane)
 IT 13274-43-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with silylbenzene oxide derivative)

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L47 ANSWER 29 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 94:121188 CASREACT
 TI Aromatization of arene 1,2-oxides. 1,2-Oxides of methyl phenylacetate and methyl trans-cinnamate
 AU Chao, Herbert S. I.; Berchtold, Glenn A.
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SO Journal of Organic Chemistry (1981), 46(6), 1191-4
 CODEN: JOCEAH; ISSN: 0022-3263

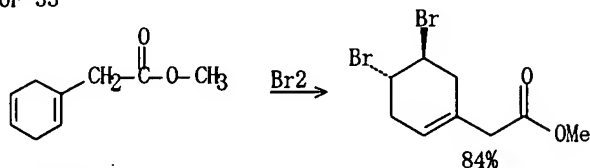
DT Journal
LA English
GI



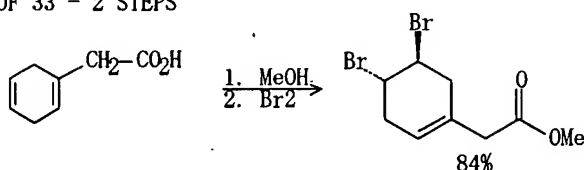
- AB Substituent migration is observed only to a minor extent during aromatization of the 1,2-oxide I (Z = CH₂) to 2-HOC₆H₄CH₂CO₂Me; the major aromatization pathway does not involve substituent migration. Substituent migration is not observed during aromatization of (E)-I (Z = CH:CH₂) to Me o-coumarate.
- CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25
- ST ring cleavage arene oxide; oxabicycloheptadiene ring cleavage
- IT Ring cleavage
(of arene 1,2-oxides)
- IT 13274-43-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reaction of, with oxabicycloheptadieneacetate)
- IT 4409-83-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(carboxymethylation of)
- IT 76251-04-2
RL: PROC (Process)
(conversion of, to acrylic acid derivative)
- IT 103-82-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroxylation of)
- IT 76250-98-1P 76251-02-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)
- IT 75996-10-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and bromination-epoxidn. of)
- IT 76251-09-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to epoxide)
- IT 76250-97-0P 76250-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debromination of)
- IT 76251-03-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrogenation of)
- IT 66223-91-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and epoxidn. of)
- IT 36696-80-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
- IT 76250-93-6P 76250-94-7P 76250-95-8P 76250-96-9P 76251-00-8P
76251-05-3P 76251-07-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring cleavage of)
- IT 27008-28-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)
- IT 22446-37-3P 76251-01-9P 76251-06-4P 76251-08-6P
RL: SPN (Synthetic preparation); PREP (Preparation)

- (preparation of)
 IT 5927-18-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with formyloxabicycloheptene)
 IT 75961-78-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tri-Me phosphonoacetate)

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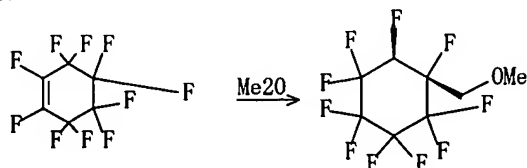
RX(21) OF 33 - 2 STEPS



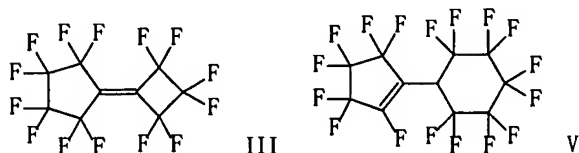
- L47 ANSWER 30 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 94:29806 CASREACT
 TI Free radical chemistry. Part 2. Additions of dimethyl ether to
 F-cycloalkenes
 AU Chambers, R. D.; Kelly, N.; Musgrave, W. K. R.; Jones, W. G. M.; Rendell,
 R. W.
 CS Dep. Chem., Univ. Sci. Lab., Durham, DH1 3LE, UK
 SO Journal of Fluorine Chemistry (1980), 16(4), 351-64
 CODEN: JFLCAR; ISSN: 0022-1139
 DT Journal
 LA English
 AB γ Ray- and peroxide-initiated addns. of Me₂O to perfluorocyclobutene
 (I), -cyclopentene and -cyclohexene give mixts. of cis and trans adducts
 in each case, with a clear preference for trans addition with I. Bromination
 of the adducts occurs selectively, but the position of chlorination
 depends dramatically on the solvent. Fluorination of the adducts with
 CoF₃ is very efficient.
 CC 22-4 (Physical Organic Chemistry)
 ST radical addn methyl ether; perfluorocycloalkene addn methoxymethyl;
 cycloalkene perfluoro addn methyl ether
 IT Bromination
 Chlorination
 Fluorination
 (of (methoxymethyl)perfluorocycloalkanes)
 IT Stereochemistry
 (of radical addition of di-Me ether with perfluorocycloalkenes)
 IT Addition reaction
 (homolytic, of di-Me ether with perfluorocycloalkenes)
 IT Cycloalkenes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (perfluoro, radical addition reaction with di-Me ether)
 IT 16520-04-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with perfluorocycloalkenes)
 IT 10026-18-3
 RL: PRP (Properties)
 (fluorinating agent, for perfluorocycloalkene adducts with di-Me ether)
 IT 76051-77-9P 76051-78-0P 76051-79-1P 76051-80-4P 76051-81-5P
 76069-73-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and fluorine-19 NMR spectrum of)

- IT 76051-82-6P 76051-83-7P 76051-84-8P 76051-85-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 355-75-9 559-40-0 697-11-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (radical addition reaction of, with di-Me ether)
 IT 115-10-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (radical addition reaction of, with perfluorocycloalkenes)

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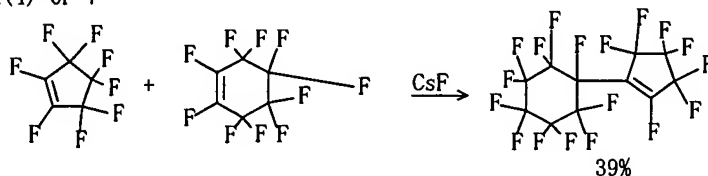
- L47 ANSWER 31 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 93:149845 CASREACT
 TI Reactions involving fluoride ion. Part 18. Derivatives of perfluoro
 cycloalkenes
 AU Chambers, Richard D.; Taylor, Graham; Powell, Richard L.
 CS Sci. Lab., Univ. Durham, Durham, DH1 3LE, UK
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and
 Bio-Organic Chemistry (1972-1999) (1980), (2), 429-34
 CODEN: JCPRB4; ISSN: 0300-922X
 DT Journal
 LA English
 GI



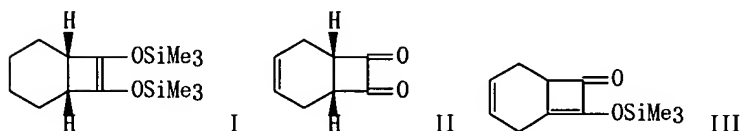
- AB F--initiated reactions of mixts. of perfluorocycloalkenes, of
 perfluorocycloalkenes with perfluoropropene, and between
 perfluorocyclobutene and perfluorobut-2-ene gave a range of oligomers.
 E.g., a mixture of perfluorocyclobutene (I) and -pentene (II) with CsF gave
 a complex mixture from which dimer III was isolated; II and
 perfluorocyclohexene (IV) with CsF gave 39% dimer V together with
 cyclopentene and cyclohexene dimers. A variation was observed in the balance
 between exo and endo isomers of perfluorocycloalkene oligomers, indicating
 that conformational interactions dominate the position of equilibrium, except
 for 4-membered rings, where angle strain is also important. Unlike I, II
 and IV do not undergo pyridine-initiated oligomerization.
 CC 24-5 (Alicyclic Compounds)
 ST fluorocycloalkene oligomerization fluoride catalysis; cycloalkene
 perfluoro oligomerization
 IT Polymerization
 (oligomerization, of perfluorocycloalkenes, fluoride-initiated)
 IT Cycloalkenes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (perfluoro, fluoride-initiated reactions of, with
 perfluorocycloalkenes)
 IT 116-15-4 355-75-9 360-89-4 559-40-0 697-11-0 68252-05-1
 68252-06-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluoride-initiated reactions of, with perfluorocycloalkene)
 IT 60983-15-5P 74693-91-7P 74693-92-8P 74693-93-9P 74693-94-0P

74693-95-1P 74693-96-2P 74693-97-3P 74693-98-4P 74693-99-5P
 74711-25-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

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L47 ANSWER 32 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
 AN 91:57096 CASREACT
 TI Bicyclo[4.2.0]oct-3-ene-7,8-dione and its mono enol silyl ether
 AU Carpino, Louis A.; Tsao, Jung-Hsien
 CS Dep. Chem., Univ. Massachusetts, Amherst, MA, 01003, USA
 SO Journal of Organic Chemistry (1979), 44(14), 2387-91
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI



AB The readily available enediol bis(trimethylsilyl) ether I is a useful intermediate in the synthesis of free bicyclo[4.2.0]oct-3-ene-7,8-dione (II) as well as a protected form, the mono enol silyl ether (III). Bromination of I gave small amts. of both II and III. If bromination was followed by addition of Et₃N, III could be obtained in 41% yield. Other products were also isolated from the bromination of I depending on the conditions. The best route to II involved the oxidative desilylation of I by means of dichlorodicyanoquinone in dioxane.

CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 24

ST bicyclooctenedione; silylbicyclooctene bromination; enol silyl ether
 IT 18014-24-9

RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidative desilylation of)

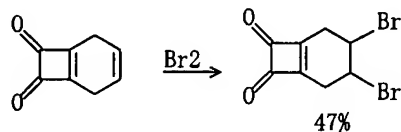
IT 6383-11-5P 56402-15-4P 70355-61-2P 70355-62-3P 70355-63-4P
 70355-64-5P 70355-65-6P 70355-66-7P 70355-67-8P 70355-68-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 7669-54-7

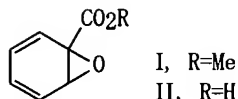
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with enediol bis(trimethylsilyl) ether)

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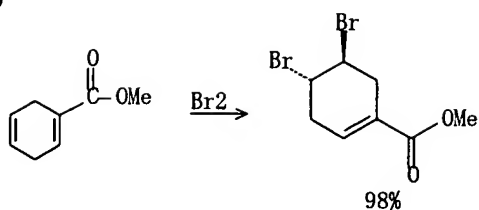
L47 ANSWER 33 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 91:19491 CASREACT
 TI Aromatization of arene 1,2-oxides. 1-Carboxy- and 1-carboalkoxybenzene oxides
 AU Boyd, Derek R.; Berchtold, Glenn A.
 CS Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SO Journal of the American Chemical Society (1979), 101(9), 2470-4
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 GI

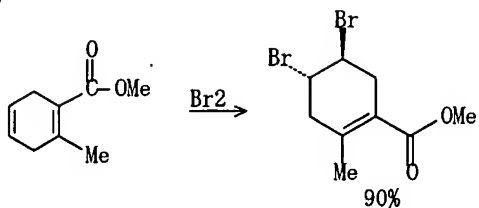


AB The reaction course for aromatization of 1-carboxy- and 1-carboalkoxybenzene oxides is established, and the importance of the 1,2-oxides of benzoic acids as intermediates in biol. hydroxylations is considered. Acid-catalyzed rearrangement of 1-carbomethoxybenzene oxide (I) and its 2-D, 2-Me, 4-Me, and 2-MeO2C derivs. occurs exclusively by an NIH shift involving migration of the carbomethoxy group. Aromatization of 1-carboxybenzene oxide (II) affords a mixture of salicylic acid and phenol, the ratio of which is pH-dependent. The 2- and 4-Me derivs. of II decarboxylate to o- and p-cresol, resp., on attempted isolation.
 CC 22-5 (Physical Organic Chemistry)
 Section cross-reference(s): 6
 ST aromatization benzoate oxide mechanism; hydroxylation biol benzoate oxide
 IT Aromatization
 (of benzoate oxides, mechanism of)
 IT Hydroxylation
 (biol., mechanism of)
 IT 60237-62-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (attempted aromatization of)
 IT 33279-97-9 50983-21-6 50983-22-7 53312-54-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of)
 IT 67490-09-9P 67490-11-3P 70588-16-8P 70588-17-9P 70588-18-0P
 70588-19-1P 70588-20-4P 70588-21-5P 70588-22-6P 70588-23-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and aromatization of)
 IT 67629-47-4P 70588-30-6P 70588-31-7P 70588-32-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and dehydrobromination of)
 IT 70588-26-0P 70588-27-1P 70588-28-2P 70588-29-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and epoxidn. of)
 IT 70588-24-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and rearrangement of)
 IT 70588-25-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

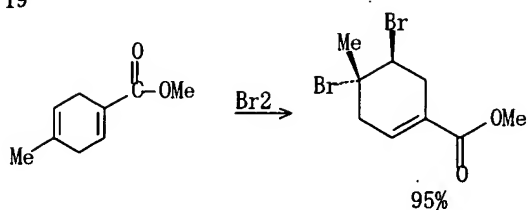
RX(12) OF 19



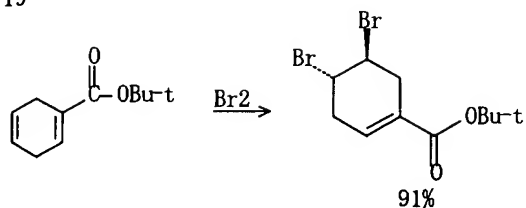
RX(13) OF 19



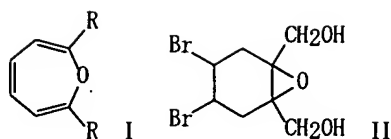
RX(14) OF 19



RX(18) OF 19

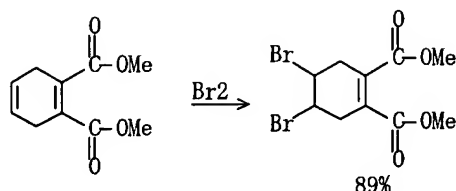


L47 ANSWER 34 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
AN 85:62929 CASREACT
TI Oxepin-2,7-dialdehyde
AU Vogel, E.; Beermann, D.; Balci, E.; Altenbach, H. J.
CS Inst. Org. Chem., Univ. Cologne, Cologne, Fed. Rep. Ger.
SO Tetrahedron Letters (1976), (15), 1167-70
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA German
GI

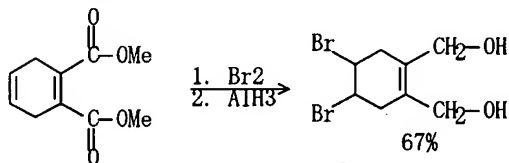


- AB The title compound (I; R = CHO) was prepared from di-Me cyclohexa-1,4-diene-1,2-dicarboxylate in 5 steps via the epoxide II. I (R = CHO) was converted by standard methods to I (R = CO₂H, CO₂Me, CN).
- CC 27-22 (Heterocyclic Compounds (One Hetero Atom))
- ST oxepindialdehyde
- IT 3479-80-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation with cycloheptatrienedialdehyde)
- IT 28172-94-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation with dibromoglutaric acid)
- IT 14309-54-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(dihydrobromination of, in oxepindialdehyde preparation)
- IT 55759-42-7P 60237-61-8P 60237-62-9P 60237-63-0P 60237-64-1P 60237-65-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 60237-56-1P 60237-57-2P 60237-58-3P 60237-59-4P 60237-60-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in oxepindialdehyde preparation)

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RX(9) OF 29 - 2 STEPS



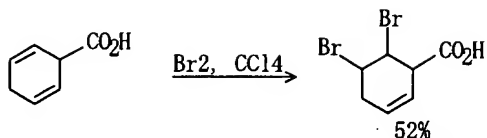
- L47 ANSWER 35 OF 36 CASREACT COPYRIGHT 2005 ACS on STN
- AN 55:137124 CASREACT
- TI 1,4-Dihydrobenzoic acid, preparation and properties
- AU Plieninger, Hans; Ege, Gunter; Jung, Friedrich; Maier-Borst, Wolfgang
- CS Univ. Heidelberg, Germany
- SO Chemische Berichte (1961), 94, 2088-95
CODEN: CHBEAM; ISSN: 0009-2940
- DT Journal
- LA Unavailable
- AB 1,4-Dihydrobenzoic acid (I) (prepared by Birch reduction of BzOH) was autoxidizable and rearranged with KOH to the 3,4-isomer (II). BzOH (60 g.) and then 240 cc. MeOH followed during 2-3 hrs. by 30 g. powdered Na added at -40 to -45° with cooling and stirring to 1.5 l. liquid NH₃, the mixture cooled to -70° and treated with 30 g. NH₄Cl, the NH₃ evaporated with stirring in vacuo below 40°, the residue treated under N carefully with 100 cc. boiled H₂O, concentrated in vacuo, diluted under N with 500 cc. H₂O, acidified with cooling and stirring with HCl, and extracted with

three 200-cc. portions Et₂O, and the extract worked up gave 52.8 g. I (containing 3% BzOH), oil. I (1 g.) in an equivalent amount of 2N NaOH treated with 1.8 g. [PhCH₂SC(NH₂)₂] Cl gave the S-benzylisothiuronium salt of I, m. 148° (aqueous MeOH). I (500 mg.) in 5 cc. AcOH absorbed during 1.5 hr. at 20° over pre-reduced 100 mg. PtO₂ slightly more than the calculated amount of H. I (undil. or in C₆H₆) treated with a stream of air deposited II; the effluent gas contained H₂O₂. p-Benzoquinone (3.9 g.) in 50 cc. dioxane and 4.5 g. I heated 2 days at 80° and cooled gave 2 g. p-C₆H₄(OH)₂, m. 171-2°; the filtrate evaporated and recrystd. from H₂O gave 3 g. BzOH, m. 119-21°. I (2.6 g.) in 15 cc. 10% aqueous Na₂CO₃ treated dropwise with stirring and cooling with 210 cc. 2.1% KMnO₄ yielded 0.3 g. BzOH. I (3 g.) in 100 cc. 10% aqueous KOH containing a slight amount of p-C₆H₄(OH)₂ refluxed 2 hrs. under N and the mixture cooled, acidified, and extracted with Et₂O gave 2.5 g. II, m. 26° (cyclohexane). I (1 g.) and 0.8 g. maleic anhydride in 10 cc. dry C₆H₆ heated 6 hrs. at 60° gave 0.8 g. adduct (III), m. 241° (H₂O). III (0.7 g.) in 100 cc. MeOH with excess CH₂N₂ yielded 0.6 g. tri-Me ester of III, m. 104° (petr. ether). I (25 g.) in 30 cc. C₆H₆ added dropwise at 50-5° to 50 g. SOCl₂ and 50 cc. C₆H₆ and the mixture heated 1 hr. at 55° and evaporated in vacuo yielded 14.5 g. 1,4-dihydrobenzoyl chloride (IV), b₁₅ 82°. IV (1.2 g.) added dropwise at 0° to 30% NH₄OH gave the amide, m. 152-4° (H₂O). Similarly was prepared 1,4-dihydrobenzanilide, m. 140-1°. I (2.5 g.) (containing 2.8% BzOH) in Et₂O treated with cooling with excess CH₂N₂-Et₂O yielded 2.1 g. Me ester (V) of I, b₁₅ 84°, n_{25D} 1.4823. I (10.4 g.) (containing 4% BzOH) in 50 cc. absolute EtOH and 1.5 cc. AcCl kept 24 hrs. at 40° gave 10 g. Et ester of I, b₁₅ 91°, n_{25D} 1.4730. V (50 g.) in 200 cc. absolute Et₂O refluxed 1 hr. with 7 g. LiAlH₄ in 300 cc. Et₂O yielded 30 g. 1,4-dihydrobenzyl alc. b₁₅ 85°, n_{25D} 1.5053; all operations were performed under N. I (2.9 g.) in 20 cc. CCl₄ treated dropwise with cooling and stirring with 11.4 cc. 2M Br-CCl₄ gave 3.5 g. 2,3-dibromo-5-cyclohexenecarboxylic acid (VI), m. 106-8° (decomposition) (Et₂O-petr. ether). VI (3 g.) stirred 10 hrs. at 20° with 20 cc. AcOH and 3 g. KOAc and the mixture centrifuged from 2.4 g. KBr and evaporated in vacuo gave BzOH. VI (2 g.) in 30 cc. MeOH ozonized at -75°, hydrogenated 3 hrs. over 10% Pd-C, filtered, and evaporated, and the oily residue dissolved in 2N NaOH and treated with 2,4-(O₂N)₂C₆H₃NHNH₂ in HCl gave the derivative of 1-formylcyclopentene, m. 205-10° (decomposition). VI (5 g.) in 300 cc. H₂O treated with stirring at 0° with 193 cc. 0.1N NaOH and the mixture kept several hrs. at 20° and extracted with Et₂O yielded 1.5 g. 2-hydroxy-3-bromo-5-cyclohexenecarboxylic acid lactone, m. 50° (petr. ether). I (4.6 g.) in 30 cc. CCl₄ treated in the presence of a small amount of Fe₂O₃ with stirring at 20° with 37 cc. 2M Br-CCl₄ gave 8 g. 2,3,5,6-tetrabromocyclohexanecarboxylic acid (VII), m. 213° (Et₂O-petr. ether). VII (1 g.) boiled 2 hrs. with 100 cc. 2N NaOH and the mixture acidified with HCl and extracted with Et₂O gave o-BrC₆H₄CO₂H, needles, m. 150° (H₂O).

- CC 10D (Organic Chemistry: Alicyclic Compounds)
 IT Isomerization
 (of 2,5-cyclohexadiene-1-carboxylic acid)
 IT Infrared spectra
 Ultraviolet and visible, spectra
 (of 2,5-cyclohexadiene-1-carboxylic acid derivs.)
 IT Pseudourea, 2-benzyl-2-thio-, compds. with 2,5-cyclohexadiene-1-carboxylic acid
 IT 4794-04-1, 2,5-Cyclohexadiene-1-carboxylic acid
 (and derivs.)
 IT 88-65-3, Benzoic acid, o-bromo-
 (formation of, from 2,3,5,6-tetrabromocyclohexanecarboxylic acid)
 IT 3217-88-7, 2,5-Cyclohexadiene-1-carbonyl chloride 15419-44-0,
 1-Cyclopentene-1-carboxaldehyde, (2,4-dinitrophenyl)hydrazone
 25372-69-4, 2,5-Cyclohexadiene-1-methanol 40002-23-1,
 1,5-Cyclohexadiene-1-carboxylic acid 64739-70-4, 2,5-Cyclohexadiene-1-
 carboxamide 98280-27-4, Cyclohexanecarboxylic acid, 2,3,5,6-tetrabromo-
 98633-00-2, 2-Cyclohexene-1-carboxylic acid, 5-bromo-6-hydroxy-,
 β-lactone 99866-12-3, Bicyclo[2.2.2]oct-5-ene-2,3,5-tricarboxylic
 acid 100712-98-9, 2,5-Cyclohexadiene-1-carboxanilide 100794-17-0,
 Benzene, (4,4-dimethylcyclohexyl)- 100972-96-1, Bicyclo[2.2.2]oct-5-ene-
 2,3,5-tricarboxylic acid, trimethyl ester 102281-34-5,
 2-Cyclohexene-1-carboxylic acid, 5,6-dibromo-

(preparation of)

RX(1) OF 3



NOTE: Classification: Bromination; "1,2-Addition"; Mono-From-Bis; #
 Conditions: Br2 CCl4 ice bath

L47 ANSWER 36 OF 36 CASREACT COPYRIGHT 2005 ACS on STN

AN 55:17671 CASREACT

TI Yields of eight isomers of benzene hexachloride

AU Kanda, Yoshiya

CS Kyushu Univ., Fukuoka

SO Journal of the American Chemical Society (1960), 82, 3085-90

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

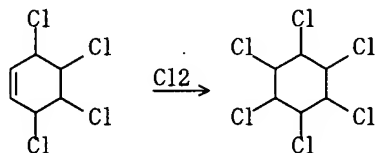
LA Unavailable

AB A simple statistical calcn. on the yields of eight isomers of benzene hexachloride was carried out. Processes of chlorination were proposed and several rate controlling factors and coefficients were estimated from data on the yields of benzene hexachloride isomers from benzene tetrachloride isomers (according to a study by Orloff, et al., CA 48, 10615f) and the principle for calculating the yields of products was applied to all the chlorination processes from benzene to benzene hexachloride, via benzene dichloride and benzene tetrachloride. The calculated values were in fairly good agreement with observed data. A reason for a rich yield of the α -isomer, a possibility of finding still unknown isomers, and a possibility of obtaining a good yield of the γ -isomer were also discussed.

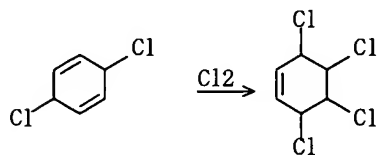
CC 10E (Organic Chemistry: Benzene Derivatives)

IT 608-73-1, Cyclohexane, 1,2,3,4,5,6-hexachloro-
 (preparation of)

RX(1) OF 6



RX(2) OF 6



NOTE: Classification: Chlorination; "1,2-Addition"; Mono-From-Bis; #
 Conditions: Cl2; # Comments: no catalyst used

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FILE 'HOME' ENTERED AT 14:57:16 ON 03 MAY 2005

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